Office of the Secretary Of Defense (OSD)
Assistant Secretary of Defense (Research & Engineering)
12.B Small Business Technology Transfer (STTR)
Proposal Submission Instructions

Introduction

The Assistant Secretary of Defense (Research & Engineering) STTR Program is sponsoring seven topics in the Critical Materials Technology Focus Area and one in Information Assurance in the Cyber Domain Technology Focus Area, for a total of eight topics in this solicitation.

The Army, Navy and Air Force are participating in the OSD STTR program. The service laboratories act as OSD's Agent in the management and execution of the contracts with small businesses.

In order to participate in the OSD STTR Program, all potential proposers should register on the DoD SBIR/STTR Web site at https://www.dodsbir.net/submission as soon as possible. Follow the instructions for electronic submittal of proposals. It is required that all proposers submit their proposal electronically through the DoD SBIR/STTR Proposal Submission Website at https://www.dodsbir.net/submission. If you experience problems submitting your proposal, call the SBIR/STTR Help Desk (toll free) at 1-866-724-7457.

Refer to Section 1.5 of the DoD Program Solicitation for the process of submitting questions on STTR and Solicitation Topics. During the Pre-release period proposers have an opportunity to contact topic authors by telephone or e-mail to ask technical questions about specific solicitation topics, however, proposal evaluation is conducted only on the written proposal. Contact during the Pre-release period is considered informal, and will not be factored into the selection for award of contracts. Contact with the topic authors by telephone or e-mail subsequent to the Pre-release period is prohibited. To obtain answers to technical questions during the formal Solicitation period, please visit http://www.dodsbir.net/sitis. Refer to the front section of the solicitation for the exact dates.

OSD WILL NOT accept any proposals that are not submitted through the on-line submission site. The submission site does not limit the overall file size for each electronic proposal; but there is only a **25-page limit**. File uploads may take a great deal of time depending on your file size and your internet server connection speed. If you wish to upload a very large file, it is highly recommended that you submit prior to the deadline submittal date, as the last day is heavily trafficked. You are responsible for performing a virus check on each technical proposal file to be uploaded electronically. The detection of a virus on any submission may be cause for the rejection of the proposal.

Firms with strong research and development capabilities in science or engineering in any of the topic areas described in this section and with the ability to commercialize the results are encouraged to participate. Subject to availability of funds, the ASD(R&E) STTR Program will support high quality research and development proposals of innovative concepts to solve the listed defense-related scientific or engineering problems, especially those concepts that also have high potential for commercialization in the private sector. Objectives of the ASD(R&E) STTR Program include stimulating technological innovation, strengthening the role of small business in meeting DoD research and development needs, fostering and encouraging participation by minority and disadvantaged persons in technological innovation, and increasing the commercial application of DoD-supported research and development results. The guidelines presented in the solicitation incorporate and exploit the flexibility of the SBA Policy Directive to encourage proposals based on scientific and technical approaches most likely to yield results important to DoD and the private sector.

Proposal Submission

Refer to Sections 3.0 and 6.0 of the DoD Program Solicitation for program requirements and proposal submission instructions. Proposals shall be submitted in response to a specific topic identified in the following topic description sections. The topics listed are the only topics for which proposals will be accepted. Scientific and technical information assistance may be requested by using the SBIR/STTR Interactive Technical Information System (SITIS). OSD's technical proposal page limit is 25 pages.

Proposer Eligibility

Each proposer must qualify as a small business for research or research and development purposes as defined in Section 2.0 and certify to this on the Cover Sheet of the proposal. In addition, a minimum of 40% of each STTR project must be carried out by the small business concern and a minimum of 30% of the effort performed by the research institution, as defined in Section 2.8. The percentage of work is usually measured by both direct and indirect costs, although proposers planning to subcontract a significant fraction of their work should verify how it will be measured with their DoD contracting officer during contract negotiations. For both Phase I and II, the principal investigator must be primarily employed with the small business firm or the research institution. At the time of award of a Phase I or Phase II contract, the small business concern must have at least one employee in a management position whose primary employment is with the small business and who is not also employed by the research institution. Primary employment means that more than one half (50%) of the employee's time is spent with the small business. Primary employment with a small business concern precludes full-time employment at another organization. For both Phase I and Phase II, all research or research and development work must be performed by the small business concern and its subcontractors in the United States. Deviations from the requirements in this paragraph must be approved in writing by the contracting officer (during contract negotiations).

A small business concern must negotiate a written agreement between the small business and the research institution allocating intellectual property rights and rights to carry out follow-on research, development, or commercialization (see Model Agreement for the Allocation of Rights).

Joint ventures and limited partnerships are permitted for the small business portion, provided that the entity created qualifies as a small business in accordance with the Small Business Act, 15 USC 631, and the definition below.

Definition of a Small Business

A small business concern is one that, at the time of award of Phase I and Phase II, meets all of the criteria established by the Small Business Administration which are published in 13 C.F.R § 121.701-705, repeated here for clarity. A small business concern is one that, at the time of award of Phase I and Phase II, meets all of the following criteria:

a. Is independently owned and operated, is not dominant in the field of operation in which it is proposing, has a place of business in the United States and operates primarily within the United States or makes a significant contribution to the US economy, and is organized for profit.

b. Is (a) at least 51% owned and controlled by one or more individuals who are citizens of, or permanent resident aliens in, the United States, or (b) it must be a for-profit business concern that is at least 51% owned and controlled by another for-profit business concern that is at least 51%

owned and controlled by one or more individuals who are citizens of, or permanent resident aliens in, the United States.

c. Has, including its affiliates, an average number of employees for the preceding 12 months not exceeding 500, and meets the other regulatory requirements found in 13 CFR Part 121. Business concerns are generally considered to be affiliates of one another when either directly or indirectly,

(a) one concern controls or has the power to control the other; or (b) a third-party/parties controls orhas the power to control both.

Control can be exercised through common ownership, common management, and contractual relationships. The term "affiliates" is defined in greater detail in 13 CFR 121.103. The term "number of employees" is defined in 13 CFR 121.106.

A business concern may be in the form of an individual proprietorship, partnership, limited liability company, corporation, joint venture, association, trust, or cooperative. Further information may be obtained at http://sba.gov/size or by contacting the Small Business Administration's Government Contracting Area Office or Office of Size Standards.

Description of the OSD STTR Three Phase Program

Phase I is to determine, insofar as possible, the scientific or technical merit and feasibility of ideas submitted under the STTR Program and will typically be one half-person year effort over a period not to exceed six months, with a dollar value up to $100,000. OSD plans to fund three Phase I contracts, on average, and downselect to one Phase II contract per topic. This is assuming that the proposals are sufficient in quality to fund this many. Proposals are evaluated using the Phase I evaluation criteria, in accordance with Section 4.2 of the DoD Program Solicitation. Proposals should concentrate on that research and development which will significantly contribute to proving the scientific and technical feasibility of the proposed effort, the successful completion of which is a prerequisite for further DoD support in Phase II. The measure of Phase I success includes technical performance toward the topic objectives and evaluations of the extent to which Phase II results would have the potential to yield a product or process of continuing importance to DoD and the private sector, in accordance with Section 4.3 of the DoD Program Solicitation.

Subsequent Phase II awards will be made to firms on the basis of results from the Phase I effort and the scientific and technical merit of the Phase II proposal in addressing the goals and objectives described in the topic. Phase II awards will typically cover two to five person-years of effort over a period generally not to exceed 24 months (subject to negotiation) with a dollar value up to $750,000. Phase II is the principal research and development effort and is expected to produce a well defined deliverable prototype or process. A more comprehensive proposal will be required for Phase II.

For Phase II, no separate solicitation will be issued. Only firms awarded Phase I contracts, and have successfully completed their Phase I efforts, may be invited to submit a Phase II proposal. Invitations to submit Phase II proposals will be released approximately at the end of the Phase I period of performance. The decision to invite a Phase II proposal will be made based upon the success of the Phase I contract to meet the technical goals of the topic, as well as the overall merit based upon the criteria in Section 4.3. DoD is not obligated to make any awards under Phase I, II, or III. For specifics regarding the evaluation and award of Phase I or II contracts, please read the front section of this solicitation very carefully. Phase II proposals will be reviewed for overall merit based upon the criteria in Section 4.3 of this solicitation.

Under Phase III, the DoD may award non-STTR funded follow-on contracts for products or processes, which meet the component mission needs. This solicitation is designed, in part, to encourage the conversion of federally sponsored research and development innovation into private sector applications. The small business is expected to use non-federal capital to pursue private sector applications of the research and development.

This solicitation is for Phase I proposals only. Any proposal submitted under prior STTR solicitations will not be considered under this solicitation; however, offerors who were not awarded a contract in response to a particular topic under prior STTR solicitations are free to update or modify and submit the same or modified proposal if it is responsive to any of the topics listed in this section.

Phase II Plus Program

The OSD STTR Program has a Phase II Plus Program, which provides matching STTR funds to expand an existing Phase II contract that attracts investment funds from a DoD acquisition program, a non-SBIR/non-STTR government program or Private sector investments. Phase II Plus allows for an existing Phase II OSD STTR contract to be extended for up to one and a half year per Phase II Plus application, to perform additional research and development. Phase II Plus matching funds will be provided on a one-for-one basis up to a maximum $500,000 of STTR funds. All Phase II Plus awards are subject to acceptance, review, and selection of candidate projects, are subject to availability of funding, and successful negotiation and award of a Phase II Plus contract modification. The funds provided by the DoD acquisition program or a non-SBIR/non-STTR government program must be obligated on the OSD Phase II contract as a modification prior to or concurrent with the OSD STTR funds. Private sector funds must be deemed an “outside investor” which may include such entities as another company, or an investor. It does not include the owners or family members, or affiliates of the small business (13 CFR 121.103).

Fast Track Policy

The Fast Track provisions in Section 4.5 of this solicitation apply as follows. Under the Fast Track policy, STTR projects that attract matching cash from an outside investor for their Phase II effort have an opportunity to receive interim funding between Phases I and II, to be evaluated for Phase II under an expedited process, and to be selected for Phase II award provided they meet or exceed the technical thresholds and have met their Phase I technical goals, as discussed in Section 4.5. Under the Fast Track Program, a company submits a Fast Track application, including statement of work and cost estimate, within 120 to 180 days of the award of a Phase I contract (see the Fast Track Application Form on www.dodsbir.net/submission). Also submitted at this time is a commitment of third party funding for Phase II. Subsequently, the company must submit its Phase I Final Report and its Phase II proposal no later than 210 days after the effective date of Phase I, and must certify, within 45 days of being selected for Phase II award, that all matching funds have been transferred to the company. For projects that qualify for the Fast Track (as discussed in Section 4.5), DoD will evaluate the Phase II proposals in an expedited manner in accordance with the above criteria, and may select these proposals for Phase II award provided: (1) they meet or exceed selection criteria (a) and (b) above and (2) the project has substantially met its Phase I technical goals (and assuming budgetary and other programmatic factors are met, as discussed in Section 4.1). Fast Track proposals, having attracted matching cash from an outside investor, presumptively meet criterion (c). However, selection and award of a Fast Track proposal is not mandated and DoD retains the discretion not to select or fund any Fast Track proposal.

Follow-On Funding

In addition to supporting scientific and engineering research and development, another important goal of the program is conversion of DoD-supported research and development into commercial products. Proposers are encouraged to obtain a contingent commitment for private follow-on funding prior to Phase II where it is felt that the research and development has commercial potential in the private sector. Proposers who feel that their research and development have the potential to meet private sector market needs, in addition to meeting DoD objectives, are encouraged to obtain non-federal follow-on funding for Phase III to pursue private sector development. The commitment should be obtained during the course of Phase I performance. This commitment may be contingent upon the DoD supported development meeting some specific technical objectives in Phase II which if met, would justify non-federal funding to pursue further development for commercial purposes in Phase III. The recipient will be permitted to obtain commercial rights to any invention made in either Phase I or Phase II, subject to the patent policies stated elsewhere in this solicitation.

The following pages contain a summary of the technology focus areas, followed by the topics.

Critical Materials Technology Area Topics

The Office of the Secretary of Defense is interested in innovative, collaborative research associated with the broad area of strategic and critical materials. The Department of Defense (DoD) relies on many products that incorporate materials that are not found or produced in sufficient quantities domestically to meet potential crucial defense needs. The DoD, therefore, is interested in research that increases the potential domestic or otherwise secure supply of such materials or reduces reliance on them. General research areas of significance include substitution or reduction concepts, advanced ore dressing or processing to increase recovery and reduce environmental impact, and advanced or more efficient means of recovery from products and recycling. Research may include efforts dealing with materials synthesis, processing, fabrication, or design that leads to reduction in the reliance on strategic and critical materials. Of additional interest is research that improves the ability to model and understand the supply and value chains associated with materials from the ground through a whole life-cycle.

The Critical Materials Technology Topics are:

OSD12-T01	Advanced Separation Technologies for Extraction of Rare Earth Elements (REE)
OSD12-T02	Novel Primary Processing of Scarce Element Ores
OSD12-T03	Novel Electrolytic Extraction Processes for Scarce Elements
OSD12-T04	Efficient, Environmentally-Compatible Recovery Technologies for Rhenium and Other Strategic Critical Materials
OSD12-T05	Theory-Driven Protocols for Replacing Elemental Composition of Strategic Materials
OSD12-T06	Sustainable Alloy Design: Rare Earth Materials Challenge
OSD12-T07	HIGH STRENGTH AND TOUGHNESS TUNGSTEN CARBIDE (WC) WITH NON-COBALT (Co) MATRICES

Information Assurance in the Cyber Domain Technology Focus Area

To take advantage of rapid technological advances in industry, DoD systems make extensive use of commercial off-the-shelf (COTS) hardware and software. These gains, however, come at the price of creating systems that are ever-more complex, harder to make secure, and based on information technology that is equally available for adversaries to examine for vulnerabilities and means of compromise. Furthermore, avenues of approach are available to adversaries to exploit vulnerabilities through interconnected networks and through the global supply chain for commercial technologies.

The goal in the cyber domain is to develop techniques for ensuring trust, resiliency, and agility, and to assure that missions for which the DoD relies on information technology can be conducted successfully despite incessant attempted incursions and even successful cyber attacks on the underlying technologies and systems. An important additional challenge for the areas mentioned above is that of understanding and validating the effectiveness of the techniques at scale, to inform the further development and improvement of the technologies and to guide their operational use.

The DoD seeks to develop ways of building features and architectural provisions into hardware, system software, and applications that make systems and networks more difficult to damage, more maneuverable to move out of the path of attacks, and more able to withstand damage and still perform their functions. The successful operation of the DoD's systems must not depend upon preventing or detecting every cyber attack in order to counter it. Networked systems must persevere, contain effects of incursions, blunt and frustrate attacks, and allow us to hunt and isolate adversaries within our networks, at Internet speeds. One key aspect of successful cyber defense is to enhance the effectiveness of cyber analysis and to increase the performance, especially at the team level, of cyber defenders. This requires a clear definition of cyber situational awareness effectiveness and expertise. Further, using the effectiveness and expertise metrics, new tools that provide real and meaningful measurement of analysts performance help us to optimize the use of human capitals (which has been the most costly part of cyber defense), and to identify opportunities to train and enhance performance of less experienced analysts.

The Information Assurance Technology in the Cyber Domain topic is:

OSD12-T08 Effective Cyber Situation Awareness (CSA) Assessment and Training

OSD STTR 12.B Topic Index

OSD12-T01	Advanced Separation Technologies for Extraction of Rare Earth Elements (REE)
OSD12-T02	Novel Primary Processing of Scarce Element Ores
OSD12-T03	Novel Electrolytic Extraction Processes for Scarce Elements
OSD12-T04	Efficient, Environmentally-Compatible Recovery Technologies for Rhenium and Other Strategic Critical Materials
OSD12-T05	Theory-Driven Protocols for Replacing Elemental Composition of Strategic Materials
OSD12-T06	Sustainable Alloy Design: Rare Earth Materials Challenge
OSD12-T07	HIGH STRENGTH AND TOUGHNESS TUNGSTEN CARBIDE (WC) WITH NON-COBALT (Co) MATRICES
OSD12-T08	Effective Cyber Situation Awareness (CSA) Assessment and Training

OSD STTR 12.B Topic Descriptions

OSD12-T01 TITLE: Advanced Separation Technologies for Extraction of Rare Earth Elements (REE)

TECHNOLOGY AREAS: Materials/Processes

OBJECTIVE: The objective of this research is to conduct fundamental surface chemistry measurements and demonstrate the use of these data to laboratory and small scale froth flotation systems so that more effective recovery can be achieved than with existing methods.

DESCRIPTION: A critical step in the extraction of elements from ore, especially rare earth elements that are found in complex minerals, is separation. Froth flotation is a highly versatile method for physically separating particles based on differences in the ability of air bubbles to selectively adhere to specific mineral surfaces in a mineral/water slurry. The particles with attached air bubbles are then carried to the surface and removed, while the particles that remain are completely wetted stay in the liquid phase. Froth flotation is an attractive approach, but its effectiveness is limited for the rare earth minerals as they occur as phosphates, carbonates, fluorides, silicates and oxides with gangue minerals, which often share physical properties. By providing another tool for separation, increased understanding of localized surface chemistries in complex rare earth minerals could enable affordable processes that improve grades, recoveries, capital costs and operating costs for separation of rare earth elements from their ores. The techniques used to characterize surface chemistry in flotation relate to methods to make selective minerals hydrophobic by adjusting the surface charge so that ionic collectors may be adsorbed. In the case of non-sulfide minerals this is complicated by the fact that the waste materials are also non-sulfide, so very small differences in surface chemistry properties are observed. Finding chemical methods to selectively adsorb collectors onto the desired minerals requires additional fundamental understanding of the surface ions (potential determining ions) and charges (electrochemical potentials) encountered. The work, coupled with the development of a fundamental understanding can lead to greatly improved processes for concentration by froth flotation.

PHASE I: In the phase I effort, the investigators need to explore the fundamental surface chemistry measurements (zeta potential, contact angle, micro-flotation tests) on pure rare earth mineral samples to evaluate various alternatives chemistries for selective froth flotation. Pure mineral samples need to be acquired, crushed, ground, screened, and analyzed using chemical and X-ray diffraction techniques. The surface chemistry measurements will be made as a function of collector type, pH, feed rate, particle size, mineral composition (phosphate, carbonate, fluoride, oxide, silicate), surface modification chemicals, etc. Attention will also be paid to the principal gangue minerals that occur in these ore bodies. Models are to be developed to describe and understand the surface chemistry and relate this to separation efficiency. Process environmental impact will also be a factor of evaluation.

PHASE II: In the phase II effort, the investigators shall evaluate and validate the process models, modify the process models and analyze and characterize the efficiency and the environmental impact of the separation methodology using real crushed ores using standard large scale laboratory flotation equipment. Modification of the models, as necessary, based on the test results, will be conducted and retested to determine the range of their applicability. This will demonstrate the effect of this increased understanding on the grades and recoveries obtained by determining (1) the Ratio of Concentration and (2) the Percent REE Recovered. This then could be compared to conventional methods in order to demonstrate increased value and/or reduced operating costs as a function of ore type and original concentration. Separation variability as a function of REE ore composition should be assessed. If viable, scalability will be evaluated and preliminary drawings of pilot plant floth floatation system will be planned.

PHASE III: Working with industry, a pilot plant sized floth floatation system is constructed and various crushed commercial ores will feed to determine separation efficiency based on (1) the Ratio of Concentration and (2) the Percent REE Recovered.

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: The modeling of surface chemistries for froth floatation will lead to greater separation efficiencies and benefit the domestic mineral extractive companies specializing in rare earth recovery and production. More secure, domestic REE sources would be of great strategic importance to the Department of Defense for many applications where REE are utilized.

REFERENCES:
1. Q. Min, Y.Y. Duan, X.F. Peng, A.S. Mujumdar, C. Hsu, "Froth Flotation of Mineral Particles: Mechanism", Drying Technology, v. 26 (8), 985-995 (2008).

2. S. Farrokhpay, "The Significance of Froth Stability in Mineral Flotation – A Review", Advances in Colloid and Interface Science, v. 166 (1-2) 1-7 (2011).

3. N. Barbian, E. Ventura-Medina, J.J. Cilliers, "Dynamic Froth Stability in Froth Flotation", v. 16(11), 1111-1116 (2003).

KEYWORDS: froth floatation, surface chemistry, rare earth separation, ore separation, recovery, hydrophilic, hydrophobic, wetting, air bubbles

OSD12-T02 TITLE: Novel Primary Processing of Scarce Element Ores

TECHNOLOGY AREAS: Materials/Processes

OBJECTIVE: The objective of this project is to develop and demonstrate at a relevant laboratory scale a novel, efficient, and environmentally friendly approach to the extraction, concentration, and separation of rare-earth elements from common ore stocks. This project supports the goals of the Materials Genome Initiative (MGI) in the area of Integrated Computational Materials Engineering (ICME).

DESCRIPTION: The rare-earth elements find uses in hundreds of high tech applications, including cellular telephones, laptop computers, iPods, critical military applications, and green technologies. These reactive metals have a natural abundance that is similar to that of copper. Their high costs and relative scarcity are due to the high cost of their separation, concentration, and extraction from the ores. Current methods involve the leaching of the rare-earth elements from the ore, solvent ion-exchange reactions to concentrate the elements, followed by roasting. From this concentrated state, reduction using an adaptation of the Kroll process, that is the formation of halide gasses from the oxides followed by reduction using an alkali metal, is typical.

The environmental issues behind the mining of rare-earth elements are also a concern. Using concentrated sulfuric acid leaching with high temperature calcination techniques, producing one ton of calcined rare earth ore generates: up to 12,000 m3 of waste gas containing ore dust concentrate, hydrofluoric acid, sulfur dioxide, and sulfuric acid; along with approximately 75 m3 of acidic wastewater; plus up to one ton of radioactive wet waste residue. Many ores contain Thorium, a radioactive element; so that the ore dust effluents, and residuals, are radioactive and contain many toxic heavy metals. Without special treatments, these waste products pose the threat of contaminating local water supplies and producing far-field environmental damage. The disposal of tailings, the components of the ore left behind after rare-earth extraction, also contributes to the problem. Most operations simply place tailings in large land impoundments for storage. These also present long-term environmental challenges without special treatment.

A novel means of separation and fractionation of the multiple species in the ores, and concentrating these elements into separate streams using less-aggressive techniques environmentally, could enable the increased availability of these elements for engineering applications. Over the past decade, a number of liquid-liquid ion extraction processes for rare-earth elements have become available. These, however, involve the use of toxic organic compounds that require sophisticated handling technologies to work safely in an industrial scale extraction process. Novel chemistries for the extraction, concentration, and separation of these elements that a processing plant can implement in an environmentally benign manner would improve the availability, decrease the costs of extraction, and decrease the environmental impact of the extraction operations. The objective of this project is to develop and demonstrate a more environmentally benign technique for the extraction, concentration, and separation of rare-earth elements from ores.

PHASE I: The successful phase I project will develop and define concept chemistries, along with basic engineering evaluations of the relative suitabilities of the approaches and outlines of the likely relative environmental impacts.

PHASE II: The successful phase II project will down-select a concept extraction system from the phase I effort and perform detailed chemical engineering design on the proposed process. The investigators will show through combinations of modeling, simulation, and relevant experiments that the final design is suitable for insertion into a mining/extraction process.

PHASE III: Mining operations require the concentration, and separation of the relevant elements from the ores prior to subsequent purification and processing to final form. An efficient controllable process which is either environmentally benign, or can be easily controlled for minimal environmental impact, will decrease dramatically the overall costs associated with the extraction and enable mining and ore processing for deposits which are not currently profitable for exploitation.

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: The materials system developed in this project can play an important role in reducing the overall environmental impact and total cost of producing rare-earth compounds from ore systems. This we anticipate will increase the availability of these scarce materials, and reduce the overall costs for obtaining them. This will make significant changes in the ways that we can use these scarce materials in new designs.

REFERENCES:

1. C.K.Gupta, and N.Krishnamurthy, Extractive Metallurgy of Rare Earths, CRC Press, 2005.

2. House of Commons, Science and Technology Committee, Strategically important metals: Fifth Report of Session 2010–12, The Stationery Office Limited, London, UK, 2011.

3. “New opportunities for metals extraction and waste treatment by electrochemical processing in molten salts”, Donald R. Sadoway, Journal of Materials Research 10 (1995) 487-492.

4. “Emerging molten salt technologies for metals production”, Derek J. Fray, Journal of the Minerals, Metals and Materials Society 53 (2001) 27-31.

5. “The direct electrorefining of copper matte”, Douglas J. McKay, Journal of the Minerals, Metals and Materials Society 45 (1993) 44-48.

KEYWORDS: MGI; ICME; rare-earths; extractive metallurgy; electrolysis; environmental impact.

OSD12-T03 TITLE: Novel Electrolytic Extraction Processes for Scarce Elements

TECHNOLOGY AREAS: Materials/Processes

OBJECTIVE: The objective of this project is to design an electrode/electrolyte system for the electrolytic reduction of rare-earth and scarce metals directly from refined feedstocks. This project also supports the goals of the Materials Genome Initiative (MGI) in the area of Integrated Computational Materials Engineering (ICME).

DESCRIPTION: The rare-earth elements find uses in hundreds of high tech applications, including cellular telephones, laptop computers, iPods, critical military applications, and green technologies. These reactive metals have a natural abundance that is similar to that of copper. Their high costs and relative scarcity are due to the high cost of their separation, concentration, and extraction from the ores. Current methods involve the leaching of the rare-earth elements from the ore, solvent ion-exchange reactions to concentrate the elements, followed by roasting. From this concentrated state, reduction using an adaptation of the Kroll process, that is the formation of halide gasses from the oxides followed by reduction using an alkali metal, is typical.

The environmental issues behind the mining of rare-earth elements are also a concern. For typical extraction processing technologies, every ton of rare-earth metal produced results in as much as 9 kg of fluorine and 15 kg of possibly radioactive dust residues.

The electrolytic extraction of metals from the native ore chemistries is entering production for a number of systems. The process offers the advantage of scientific simplicity, though a number of technological issues loom important in using the process in production. Among these are the stability of the electrodes, the chemistry of the electrolyte, and the delivery of electrical power. To minimize costs and maximize utility, the use of a non-consumable anode is extremely important. Such an electrode must be capable of maintaining integrity at high temperatures in molten oxides and/or sulfides, and resistant to attack by high-activity oxygen in these conditions. Many prospective commercial operations use carbon as an anode, but it is consumed in the process to form gaseous CO2. This adds to the costs, and the environmental impact of the process. The objective of this project is to design and develop an anode material, with the associated electrolyte system, for electrolytic reduction of reactive rare-earth elements that has both the high temperature structural and chemical stability.

PHASE I: The successful phase I project will identify the conditions necessary for a successful electrode/electrolyte system. The investigators will then identify a group of electrode and electrolyte system chemistries, and show through thermokinetic models and simulations that the selected systems have a high likelihood of performing acceptably in the design.

PHASE II: The successful phase II project will perform validations of the preliminary electrode/electrolyte designs, and down-select a design for detail design work. The detail design work will require the development of thermokinetic data to predict system behavior in service, and the validation of the data and models prior to final design.

PHASE III: Mining operations, and materials recyclers, will implement this new technology system to reduce the costs and environmental impact of any new processing operations they might introduce.

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: The materials system developed in this project can play an important role in reducing the overall environmental impact and total cost of producing metal from ore systems. This we anticipate will increase the availability of these scarce materials, and reduce the overall costs for obtaining them. This will make significant changes in the ways that we can use these scarce materials in new designs.

REFERENCES:
1. C.K.Gupta, and N.Krishnamurthy, Extractive Metallurgy of Rare Earths, CRC Press, 2005.

2. House of Commons, Science and Technology Committee, Strategically important metals: Fifth Report of Session 2010–12, The Stationery Office Limited, London, UK, 2011.

3. “New opportunities for metals extraction and waste treatment by electrochemical processing in molten salts”, Donald R. Sadoway, Journal of Materials Research 10 (1995) 487-492.

4. “Emerging molten salt technologies for metals production”, Derek J. Fray, Journal of the Minerals, Metals and Materials Society 53 (2001) 27-31.

5. “The direct electrorefining of copper matte”, Douglas J. McKay, Journal of the Minerals, Metals and Materials Society 45 (1993) 44-48.

KEYWORDS: MGI; ICME; rare-earths; extractive metallurgy; electrolysis; environmental impact.

OSD12-T04 TITLE: Efficient, Environmentally-Compatible Recovery Technologies for Rhenium and Other Strategic Critical Materials

TECHNOLOGY AREAS: Air Platform, Materials/Processes

OBJECTIVE: The objective of this research is to demonstrate advanced, environmentally sound approaches to one or more of the following challenges associated with the recovery of rhenium: (1) economically sound methods to comminute superalloy scrap for subsequent selective treatment; (2) selective oxidation and volatilization to extract and recover rhenium; and (3) pyrometallurgical techniques to isolate and recover other valuable metals present in the superalloys. This solicitation focuses on rhenium only, but processes that show promise for other critical materials in addition to rhenium will be evaluated.

DESCRIPTION: Due to the limited amount of rhenium present in the earth's crust (approximately 1-2 part per billion) there is a significant benefit to be realized in recovering for reuse the rhenium from scrap material, spent catalysts, or end-of-life superalloys. Rhenium is found in molybdenum-copper porphyry deposits. If rhenium is present in ore that is processed, it will show up in the resulting molybdenum concentrate and will be retrieved in the molybdenum roasting process. Since there are no primary deposits of rhenium, the method in which it is processed is directly related to method in which molybdenum is produced. Very little rhenium is actually processed and isolated each year as compared to the millions of tons of copper and millions of pounds of molybdenum that are extracted from the same copper deposits. Opportunities exist for enhancing rhenium yield through technological improvements in discrete steps in the recovery process.

Due to rhenium's excellent high temperature properties (high creep resistance, high melting point, etc.) it is widely used as an alloying agent for high temperature applications including:

- Pt-Re petroleum reforming catalysts (20% current market use)
- Super alloys in high temperature turbine engines (70% current market use)
- Electromagnets, thermocouples, x-ray tube targets, and various others (10% current market use)

As of 2010, the USGS reports that all platinum-rhenium petroleum reforming catalysts are recycled [1]. Information on the recycling rates of the remaining 80% of rhenium products is quite limited, although it is postulated to be sufficiently lower than the Pt-Re catalyst industry. Thus, the largest area for potential research may be the recovery and subsequent reuse of the rhenium in superalloys and various rhenium containing products.

PHASE I: In the phase I effort, the investigators should assemble and evaluate thermodynamic data for rhenium recovery in a superalloy containing 3 wt% Re and 6 wt%. If thermodynamic data is available for all species of interest in a system, then equilibrium modeling can be performed to simulate the behavior of the system under conditions of interest, with the goal of evaluating new process approaches or optimizing existing approaches. This thermodynamic data consists of enthalpy, entropy, specific heat, and Gibbs energy, as well as Gibbs free energy of formation. The investigators will show the ability to model each processing step using existing or new models and software to predict optimal processing parameters for the Rhenium recovery. Full success in Phase I will produce a documented processing pathway for extraction of rhenium for superalloys or other rhenium-containing materials.

PHASE II: In the phase II effort, the investigators shall evaluate and validate the process models, acquire missing thermodynamic data if needed, modify the process models and analyze and characterize the efficiency and the environmental impact of the proposed recovery methodology. The investigators should work with a potential industrial partner interested in recovery of rhenium. The process should be evaluated and be able to show the selectivity and effectiveness of the optimized process.

PHASE III: The immediate application is for secondary metals suppliers. The investigators should connect with various users of rhenium-containing alloys and materials to provide either support services for process optimization, to license the process (processes) to allow the users to recover rhenium.

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: The modeling of extractive / recycling pathways should lead to an optimized recovery methodology for industry. This is of considerable interest to the aerospace, energy, and automotive industries.

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KEYWORDS: Rhenium, recovery, comminute, pyrometallurgical processing, oxidation and volatilization, superalloys, separation technologies

OSD12-T05 TITLE: Theory-Driven Protocols for Replacing Elemental Composition of Strategic Materials

TECHNOLOGY AREAS: Materials/Processes

OBJECTIVE: Use theory and computing to expedite discovery of new, thermodynamically stable compounds as replacements for strategic materials that contain rare, expensive or difficult to obtain elements of the periodic table.

DESCRIPTION: The angst surrounding scarce and strategic materials availability has prompted numerous workshops and policy studies focusing on what to do. Mitigating actions in the US, EU and Japan include: securing local and overseas resources, stockpiling, introducing recycling strategies, and, developing alternative materials. In the past, replacement strategies relied on locating known, well characterized materials and then engineering solutions around them, but, such replacement approaches are fraught with technological problems that often preclude success. This STTR takes a different approach to replacement strategies by focusing on new and unknown materials that are derived using theoretical tools. The purpose of this STTR is to provide a theory-based scientific framework allowing one to replace critical elements in a material (by judicious elemental selection and atomic positioning) such that the substituted material retains its original properties, or alternatively, by designing, de-novo, a completely new replacement material. The project has two inter-related parts: (i) discovery of new materials having properties comparable to those of an existing material for which replacement is needed; (ii) prediction of phase diagrams. The discovery component of this project can use high-throughput quantum screening [1], cluster expansion theory [2], informatics, or any other method capable of discovery and predicting properties of de-novo designed materials. Of special interest to this STTR project are techniques permitting a user to change the elemental composition of a material to obviate the need for expensive, rare or difficult to acquire elements of the periodic table. The second component of this project involves prediction of phase diagrams. Techniques including statistical mechanics, use of CALPHAD methodologies [3], etc., are acceptable. The computational tools used for this should be extensible and flexible enough to handle a wide range of alloys rather than a specific class or subset of alloys. This project should support the Materials Genome Initiative [4].

PHASE I: In the phase I effort the investigators should provide a proof-of-concept demonstration that the methodology selected for the discovery component of the project has the capability of identifying new compounds, as well as showing that the method has the capacity to predict several relevant properties of the material. Included in this phase I effort should be a detailed plan of how a Phase II project would be conducted and ultimately how the computational tools would be transitioned to a commercial entity.

PHASE II: In Phase II the investigators should mature the work initiated in the first phase and include the ability to predict phase diagrams. Depending upon the method(s) to be implemented this work could include developing the code for using graphics processing units (GPUs), massive parallelization on high performance clusters, developing or incorporating required databases, and so forth. Upon maturation of the project, the software should include an easy-to-use interface (preferably a GUI), along with a user's guide. The investigators should also develop the code so that it could be incorporated into more than one commercial package for general consumption, and develop a business strategy for the commercial product.

PHASE III: In phase III the investigators will transition their software or suite of software to one or more companies capable of marketing the product. In that regard the software could be integrated into an existing commercial product dedicated to Integrated Computational Materials Engineering (ICME) [5] or it may exist as a stand-alone component that supports the Materials Genome Initiative.

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: This software should allow for both military and non-military applications where new entities are to be used as replacements for materials containing rare, expensive, or difficult to acquire elements of the periodic table.

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KEYWORDS: Computer-Aided Design, Phase Diagram, Replacement Strategy

OSD12-T06 TITLE: Sustainable Alloy Design: Rare Earth Materials Challenge

TECHNOLOGY AREAS: Materials/Processes

OBJECTIVE: The objective of this basic research announcement is building the foundation for the discovery, characterization and predictability of non rare-earth containing high temperature aerospace alloys for high temperature applications. The program seeks highly innovative and nontraditional approaches that advance the fields of high temperature structural materials, and electro-physics research through the discovery and characterization of new non rare-earth containing high temperature metallic alloys that exhibit superior performance at conditions of thermomechanical and physical extremes.

DESCRIPTION: The rare earths elements (REE) are a group of 17 elements composed of scandium, yttrium, and the lanthanides. Rare earth materials play a pivotal role in high technology applications through their use in lasers, computers, photovoltaic devices, high temperature superconducting material systems and telecommunications. Rare earth magnets are among the world's strongest and are imperative in the miniaturization of high-tech applications such as miniaturized multi-gigabyte disc drives, cell phones, and other screens that employ liquid crystal or plasma display panel technology. Some of the end applications for rare earth elements include use in defense applications, such as jet fighter engines (in super alloys), missile guidance systems, antimissile defense, and space-based satellites, lasers, in superconductors and communication systems. Realization of the full potential of non rare-earth containing high temperature aerospace alloys requires, (1) tailoring and designing materials at the molecular level through crystal chemistry principles and combinatorial approaches, and elucidating the fundamental chemical and physical processes involved in materials performance, extending the understanding from the nanoscale to the collective (global) behavior at the microscale; and (2) learning how atoms and electrons move within a material under extreme loads to provide insight into the defect production and eventual evaluation into microstructural components, such as dislocations, voids, and grain boundaries. Interest domain includes the fundamental science at the interface of phases of heterogeneous structures, nanotechnology and mesotechnology efforts are focused on new architectures using crystal chemistry principles to create pathways to synthesize alloys for high temperature applications.

PHASE I: This focus area provides broad scientific challenges and will require the development of new experimental and computational tools to address the complexity of thermal and magnetic loads as they relate back to the performance of the material. This program seeks bold, new basic research that addresses the design, creation, and employment of nontraditional approaches on synthesis of novel high temperature magnetic alloys and nanostructures that take into account geometric or topological descriptors to characterize similarity and scaling between stimuli under the multi-dimensional external fields (i.e., magnetic and thermal fields) to secure revolutionary advances.

PHASE II: There is special interest in fundamental research of high temperature permanent magnets with minimized rare-earth element concentration by focusing on understanding combined thermal loads; e.g. thermal properties of the alloy as a function of temperature and magnetic field; understanding the demagnetization and damage initiation. Phase II should focus on the implementation of Phase I efforts by optimization of the energy product (BH)max is roughly the product of the coercive field Hc an saturation magnetization

PHASE III: The contractor will seek a potential demonstration of DoD relevant application(s) through a program, Advanced Technology Development, or Advanced Component Development and Prototypes project.

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: Rare earth magnets are widely used in commercial applications from primary electric traction motors for transportation to miniature electric motors for a vast array of automotive and actuator applications. Rare earth magnets are especially important in wind-power permanent magnet generators. Increasing temperature capability will assist in additional applications and efficiencies in these applications and open further commercial applications, especially in high-torque electric traction motors.

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KEYWORDS: high-temperature properties, materials, nanostructures, rare-earth magnet, thermal properties

OSD12-T07 TITLE: HIGH STRENGTH AND TOUGHNESS TUNGSTEN CARBIDE (WC) WITH NON-COBALT (Co) MATRICES

TECHNOLOGY AREAS: Materials/Processes

OBJECTIVE: Develop a tungsten carbide (WC) that contains a non-hazardous alternative(s) to cobalt (Co) while maintaining high density, hardness, strength, and fracture toughness.

DESCRIPTION: Increasing weapon lethality for the individual soldier has been a long-standing goal of the US Army. Tungsten carbide (WC) is a common material used in many small caliber armor-piercing projectiles. These projectiles act as rigid bodies during impact at 0 degrees obliquity and achieve twice the penetration depth of equivalent depleted uranium and tungsten heavy-alloy projectiles. However, at impact obliquities other than 0 degrees the performance dramatically drops due the tensile stresses imparted on the surface of the WC core by the bending moment generated upon impact [1-3]. Identification of WC materials with high strength and fracture toughness can lead to improved lethality in many weapons systems. Unfortunately the WC materials used as projectiles typically contain a cobalt (Co) matrix. While these materials have high density, hardness, strength and fracture toughness Co is a strategic and critical material that the US Department of Health and Human Services has classified as “reasonably anticipated to be a human carcinogen” in 2011 [4]. Efforts need to be initiated to indentify non-hazardous alternatives to Co that will yield WC materials with the necessary properties for use as armor-piercing projectiles.

PHASE I: Study and demonstrate the feasibility of a procedure to produce a WC material with high density (≥ 14 g/cm^3), flexure strength (≥ 3 GPa), a fracture toughness (≥ 11 MPa√m) and a minimum Knoop hardness, using a 2 kg indentation load, of 15 GPa. The WC material is not permitted to contain any additives that are deemed carcinogens or are long-term hazards to human health. The desired process must be able to produce WC material in a cylindrical rod form with a diameter of 5.56mm (± 0.008 mm). The proposer would be expected to report and if successful demonstrate a process for making a 500mm long rod without bowing while maintaining dimensional integrity over the entire length of the rod.

Building on the results of a successful Phase I effort, improve the procedure for fabricating rods of the WC composition from Phase I to further enhance the flexure strength and fracture toughness by 20% over the Phase I goals without a decrease in Knoop hardness. Quantify and qualify the performance of the WC material by generating quasi-static property data (flexure strength, fracture toughness, hardness, density) using appropriate standard procedures. Perform a cost analysis assessment for future production. Reasonable performance related goals expected to be achieved by the proposer related to the execution of this project are the demonstration of the selected WC production process through the generation and delivery of five (5) prototype WC rods 500mm long. These rods will be delivered to the US Army Research Laboratory (ARL) for evaluation. Similarly, a successful second year of this Phase II effort could be expected to demonstrate and deliver five (5) additional WC rods 500mm long as well as 25 near-net shape projectiles having a diameter of 5.56mm (± 0.008 mm) with a length and nose geometry specified by the Army POC. These rods and projectiles will be delivered to ARL for evaluation.

PHASE III: Ultimately the procedures developed during the performance of this SBIR for manufacturing WC small-arms projectiles will then be scaled and applied to other caliber projectiles such as the 7.62mm and 50 cal. This development could change the state-of-the-art for individual soldier lethality as we know it, with tremendous savings realized by the Army because of increased lethality

PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: Cemented tungsten carbide is widely used in the commercial sector for cutting tools, saw blades, wear-resistant components in industrial machinery, sporting goods, and surgical equipment. In all these applications having additional cobalt-free alternatives would be highly desirable and competitive.

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KEYWORDS: Tungsten Carbide, Armor-piercing projectiles, Fracture strength, Fracture toughness

OSD12-T08 TITLE: Effective Cyber Situation Awareness (CSA) Assessment and Training

TECHNOLOGY AREAS: Information Systems

OBJECTIVE: To develop a novel human-in-the loop simulation and assessment system that integrates various network models, attack graph visualization, low-level vulnerability information, and decision support functions for cyber situation awareness research and for assessing and enhancing team cyber situation awareness and assisting cyber analyst training.

DESCRIPTION: The recent increase in cyber attacks against United States critical assets has greatly expanded efforts to develop effective cyber defenses. A critical requirement for cyber situational awareness is to understand the overall context of network vulnerabilities, how they are interrelated, and how attackers may exploit them to penetrate deeper in the network. Human cyber analysts are an essential element in these efforts. Information overload and a concomitant lack of comprehensive cyber situation awareness are common problems that hamper the effectiveness of analysis. Technologies based on attack graph technology and operational concepts like team structure help create a common operating picture and lay a foundation for human analysts to establish cyber situation awareness. Systems that can carry out human-in-the loop simulation and cyber exercises will lead to new capabilities in assessing the effectiveness of analysts and tools they use, help enhance individual and team performance, and provide assistance in training of new analysts. The system developed under this topic will create a new capability in assessing team effectiveness and in training new analysts.

PHASE I: 1) Research and develop a novel simulation and analysis model based on a cognitive task analysis of the cyber domain that directly integrates network models, attack graph visualization, low-level vulnerability information, and decision support functions; 2) Extend existing team cognition metrics for cognitive system performance to assess tool effectiveness and cyber situation awareness 3) Evaluate the psychological validity of the tool by conducting human-in-the-loop testing.

PHASE II: 1) Develop a working cyber situation awareness simulation and assessment prototype, and establish the capability of recreating/replaying attack scenarios for analyst training and situation awareness effectiveness assessment; 2) Demonstrate the effectiveness of analyst training and assessment using the system.

PHASE III DUAL-USE COMMERCIALIZATION: Effective cyber attack mitigation is a critical capability for both the military and commercial sectors. The developed technology will be useable on both government networks and commercial networks for testing technology with humans-in-the-loop, for analyzing analysts' effectiveness, and for training new analysts. In Phase III, system effectiveness will be validated under real operational testing with human analysts. Benchmarking experiments will be carried out with human participants and with real and synthetic traffic generators and information feeds representative of actual scenarios. The developed system should be marketed as a product that can easily be deployed alongside existing systems.

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KEYWORDS: Cyber situation awareness, simulation and assessment, training