Physics of He Platelets in Materials

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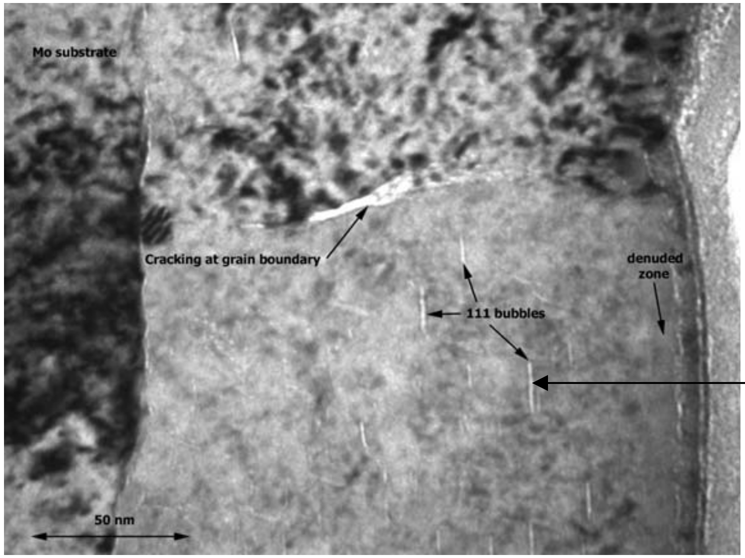
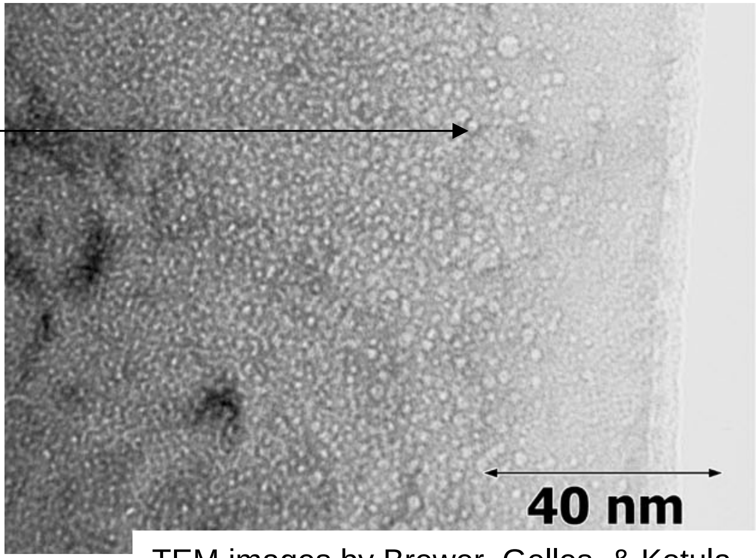
What causes the bubble shape difference?



Pd tritide

Er tritide



TEM images by Brewer, Gelles, & Kotula

Outline

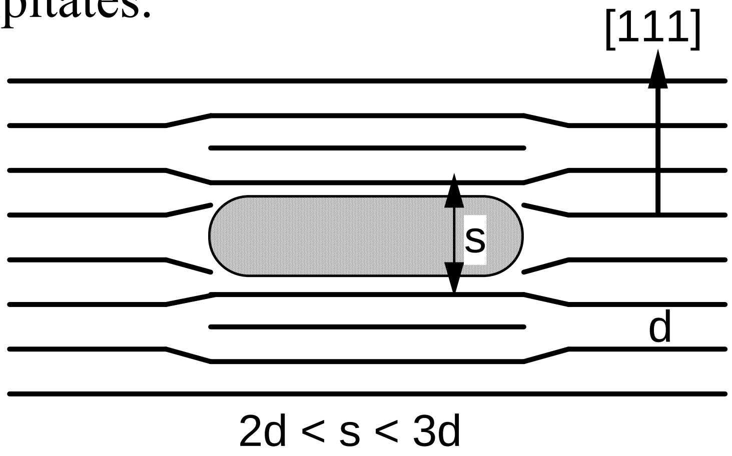
- Platelet stability and growth
- Pd vs Er system
- Testing with XRD data
- Other materials & future efforts

> *"In the spirit of a workshop, this is work in progress."*

Sandia
National
Laboratories

Thin disk-shaped He platelets can exist with dislocation dipoles.

- In FCC structures, the [111] planes provide the greatest “space” for interstitial precipitates.

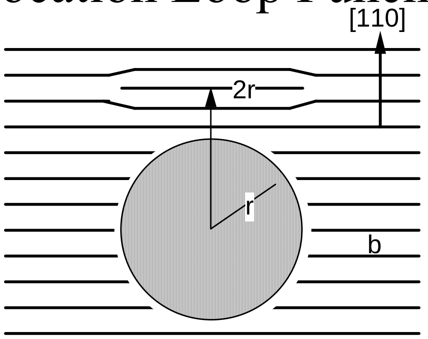


- Dislocations are formed when adjacent planes are displaced by d/2.
- The two dislocations remain attached to platelet provided adjacent (111) planes are concave toward platelet.
- The dislocations leave when the adjacent planes become straight.

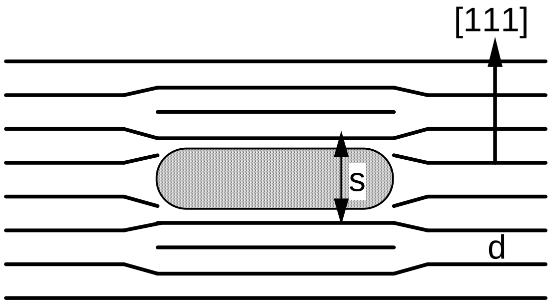
The platelets are stable if they grow by radial expansion keeping s<3d.

The pressure within the platelet has components due to surface and strain energies.

Dislocation Loop Punching:



Dislocation Dipole Expansion:



2d < s < 3d

Surface Energy: $p_e\,dV = \gamma\,dA$

$p_e\,\pi r^2\,b = \gamma\,2\pi r\,b$
$p_e = 2\gamma/r$

$p_e\,\pi[(r+b)^2-r^2]\,s = \gamma\,2\pi[(r+b)^2-r^2+(r+b)s-rs]$
$p_e = (2\gamma/s)\,[(2r+b+s)/(2r+b)]$

Lattice Strain: stress = μ strain

$p_s\,\pi r^2 = \mu\,[(b/2)/d]\,2\pi r d$
$p_s = \mu b/r$

$p_s\,\pi[(r+b)^2-r^2] = \mu\,[(d/2)/b]\,2\pi[(r+b)-r]b$
$p_s = \mu d/(2r+b)$

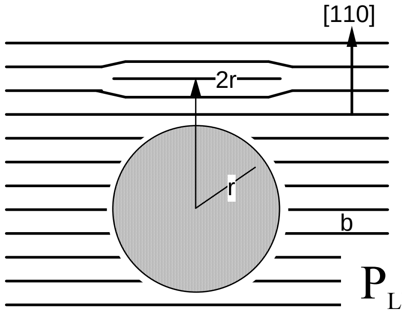
Bubble Pressure: $p = p_e + p_s$

$p_{lp} = 2\gamma/r + \mu b/r$

$p_{de} = (2\gamma/s)\,[(2r+b+s)/(2r+b)] + \mu d/(2r+b)$
$p_{de} = 2\gamma/s + \mu d/2r$, at large r

The bubble shape and growth process depend on the tritide's mechanical properties.

- Dislocation loop punching

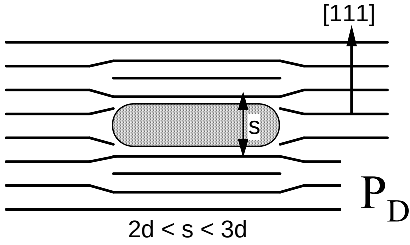


Surface Energy

Strain Energy

$$P_{LP} = 2\gamma/r + \mu b/r$$

- Dislocation dipole expansion

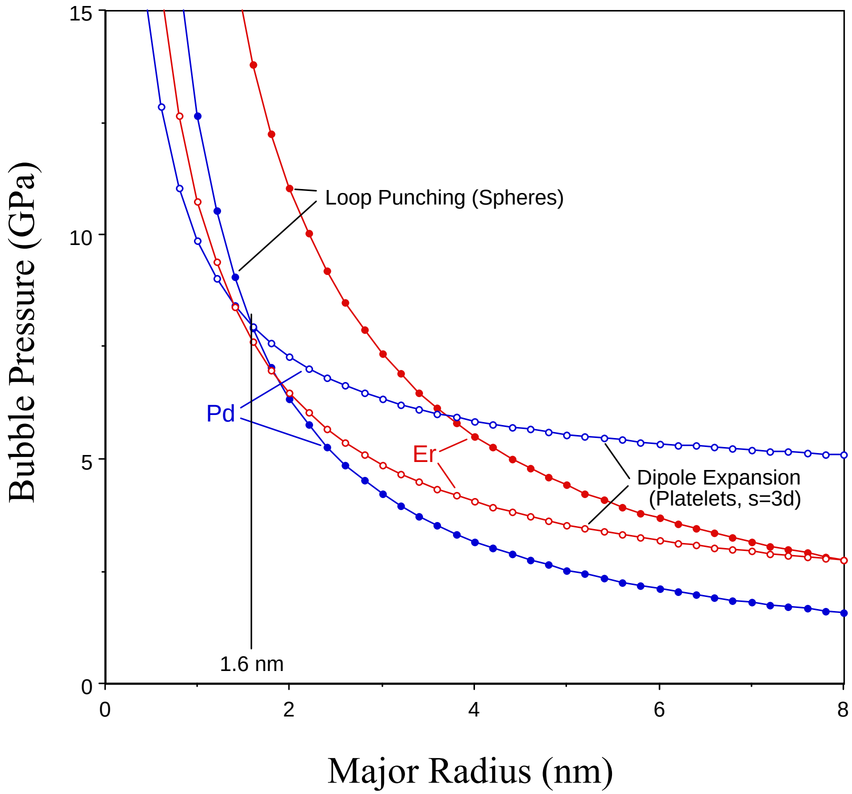


$$P_{DE} \approx 2\gamma/s + \mu d/(2r+b)$$

- Thin, disk-shaped bubbles are caused by a low surface energy (low $\gamma/\mu b$).

Note: Platelets are also the preferred shape in *young Pd tritide (<50 days).*

Tritide	γ(GPa-nm)	μ(GPa)	b(nm)	$\gamma/\mu b$
Pd	1.54	33.6	.2852	0.16
Er	0.637	57.4	.3623	0.03



This bubble shape condition holds for precipitates in a number materials.

Material	γ(GPa-nm)	μ(GPa)	b(nm)	$2\gamma/\mu b$	shape
ErT	0.637	57.4	.3623 fcc	.061	platelets
ScT	0.954	54.0	.3382 fcc	.104	early platelets, then?
TiT	1.39	76.2	.3111 fcc	.117	platelets & elongated?
Ni	1.72	76.5	.2490 fcc	.180	spheres?
ZrT	1.48	32.6	.3522 fcc	.258	spheres
PdT	1.54	33.6	.2852 fcc	.322	spheres
Be	1.10	146	.359 hex	.051	platelets
Ti-α	1.39	40.1	.291 hex	.238	platelets
W	2.22	158	.273 bcc	.103	platelets
V-α	1.95	47.4	.263 bcc	.312	spheres
Nb-α	1.90	38.2	.285 bcc	.350	spheres

- Surface energy/strain energy ratio for spherical bubbles
- Platelets are prefered for small r, where $s/2r > 2\gamma/\mu b$.

Testing of pressure formulation is provided by lattice dilation data on aged tritides.

- Tensile stress created by the precipitates produces a positive da/a.

- <u>Spherical bubbles at Loop Punching pressure:</u>
  Hydrostatic tensile stress balances bubble pressure

  $p_{LP}(\Delta V/V) = B^*(3\ da/a)_{LP}$, B^* = bulk modulus of aged material
  where $\Delta V/V = (4/3)\ \pi r^3\ n_B$, n_B = bubbles/cm^3

  $$(da/a)_{LP} = p_{LP}(\Delta V/V)\ /\ 3B^*,$$

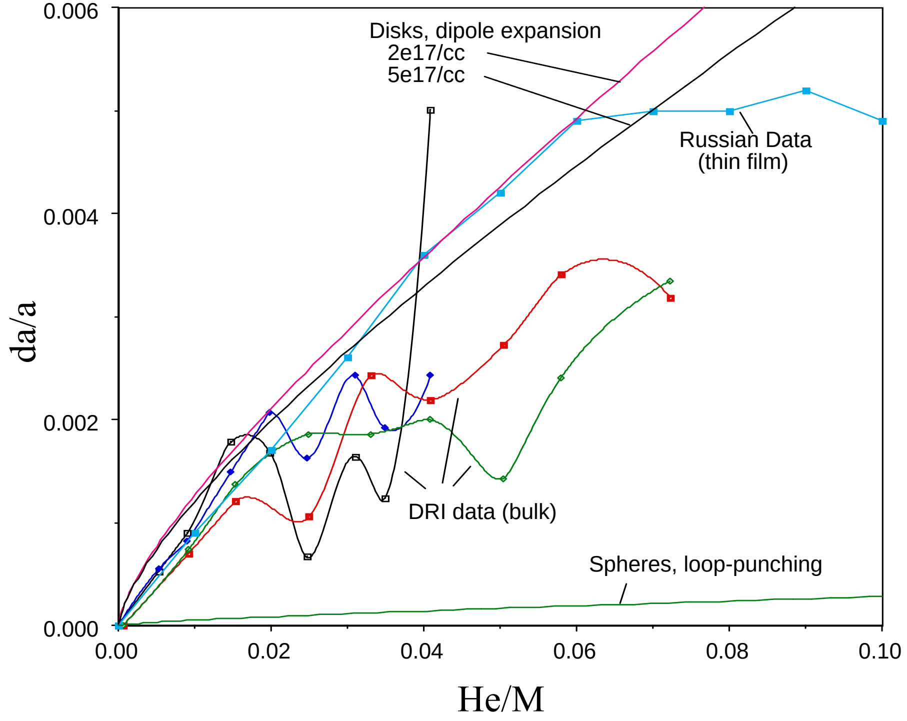
- <u>Platelets at Dipole Expansion pressure:</u>
  [111] tensile stress balances platelet pressure, 4 components
  Projection along [100] cubic axes = $1/\sqrt{3}$

  $p_{DE}(\Delta A/A)\ 4/\sqrt{3} = E^*(da/a)_{DE}$, E^* = Young's modulus of aged material
  where $\Delta A/A = \pi r^2\ (n_B/4)^{2/3}$, n_B=bubbles/cm^3

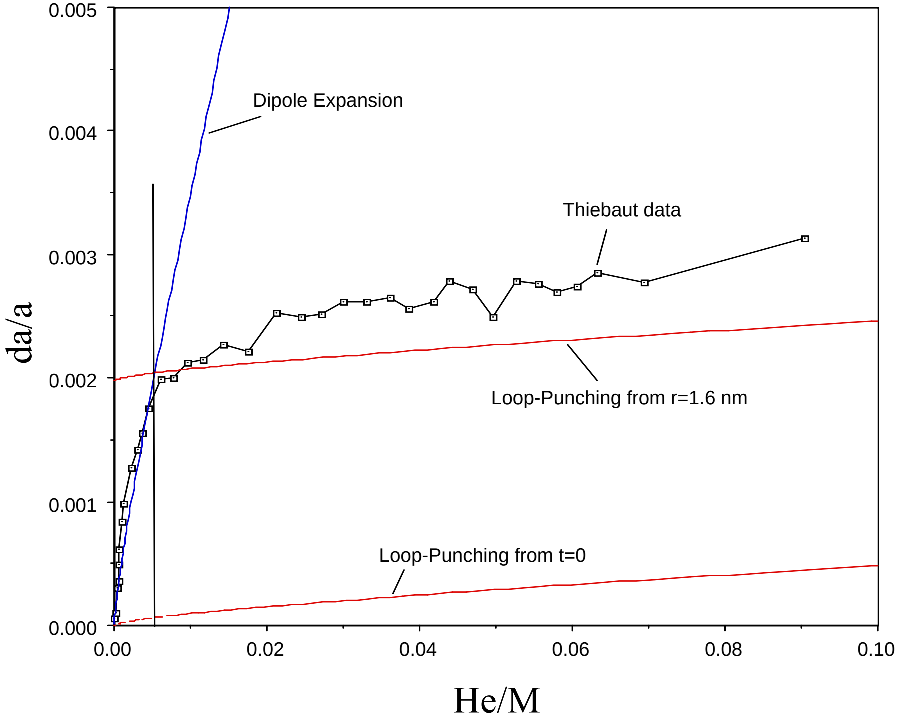
  $$(da/a)_{DE} = 4\ p_{DE}(\Delta A/A)\ /\ E^*\sqrt{3}$$

Lattice dilation data for both ErT and PdT show the effects of rapid platelet growth.

Er Tritide



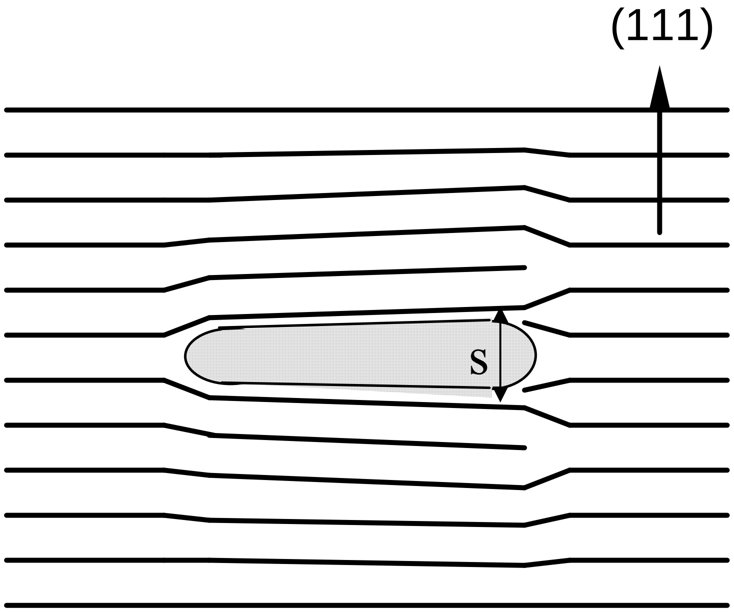
Pd Tritide



- Neither can be explained by dislocation loop punching alone.
- The model produces the correct transition point for the Pd system.
- How are platelets formed?

Transition of a nano-crack to a platelet can begin with a dislocation near the crack tip.

$PdT_{0.6}$ aged 3 months

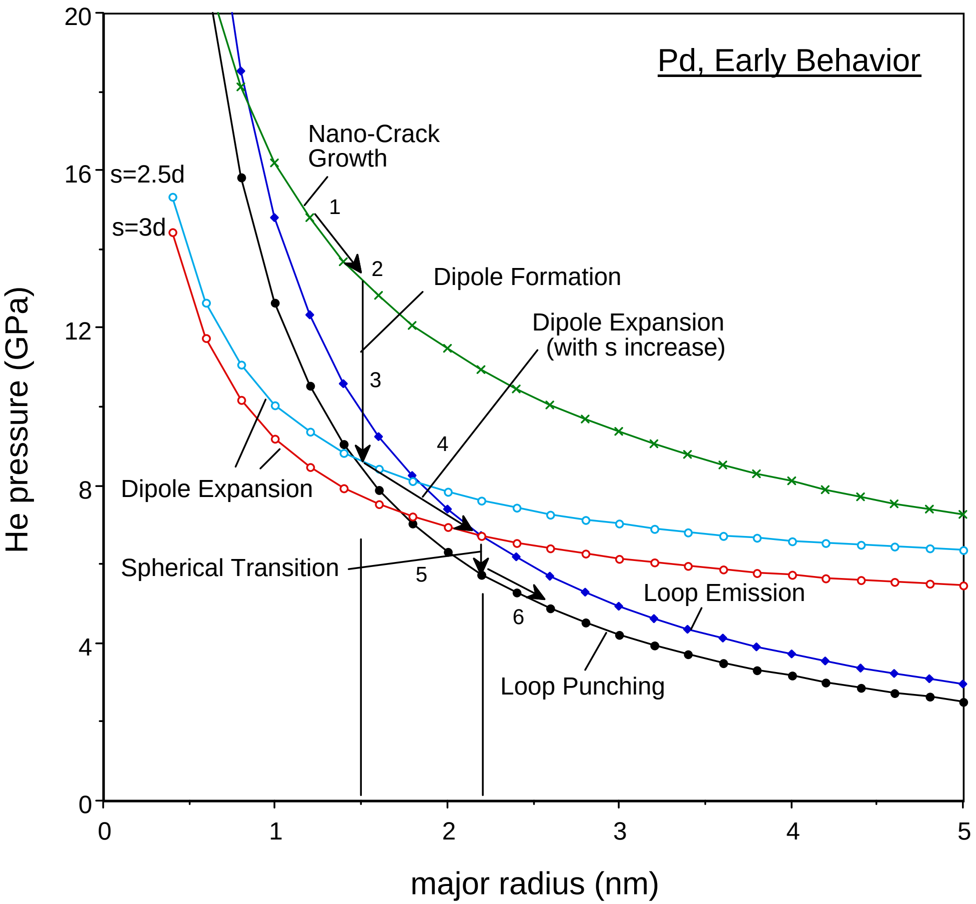


s ≈ 2d = 0.47 nm

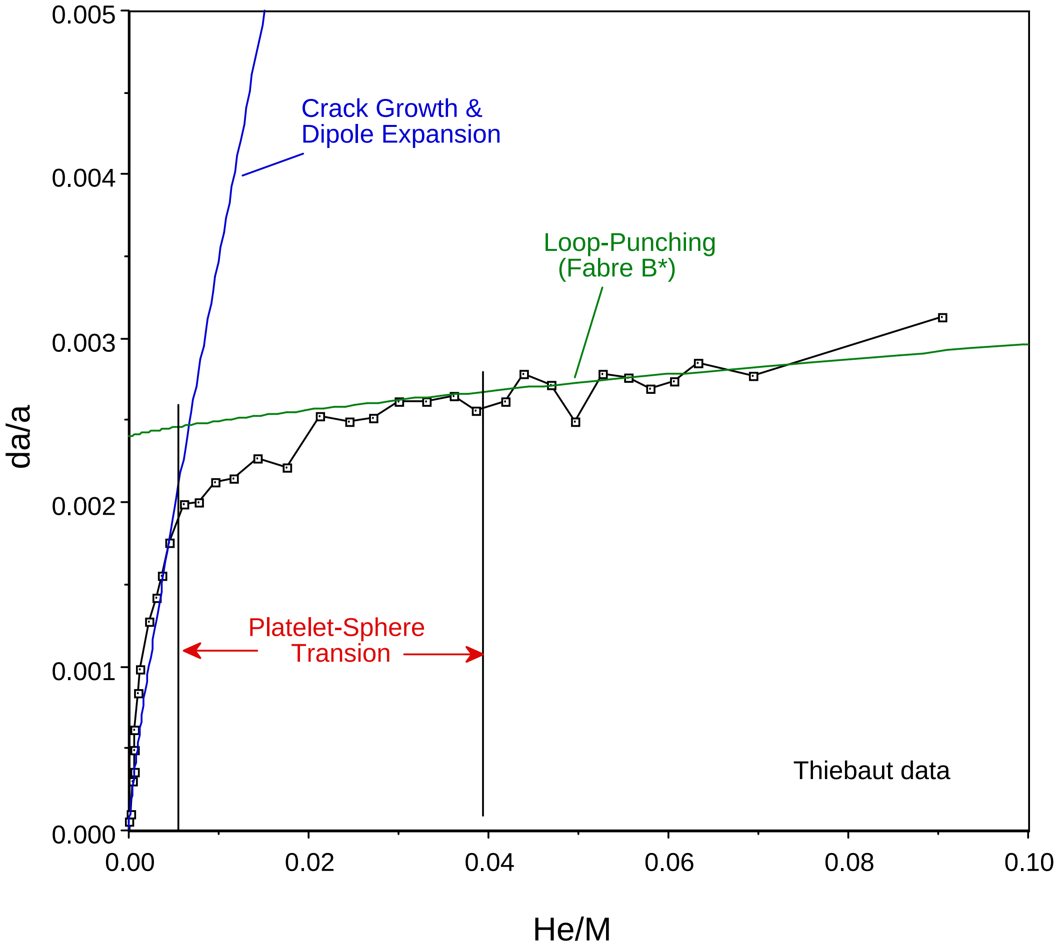
HR-TEM [110] view (Thiebaut)

The early growth of bubbles in PdT appears to have several stages.

1. He atoms collect in (111) planes and open nano-cracks (Griffith):
   $P_{nC} = 4\gamma/s$, $s = 4[\gamma(1-\nu)r/\pi\mu]^{1/2}$.
2. Dislocation dipoles form when the nano-crack gap reaches s=2d.
3. Platelet pressures drop as their thicknesses increase to s≈2.5d.
4. The platelets expand radially until s=3d, where the dipole escapes.
5. [110] loops are emitted as the platelets transition to spheres.
6. Spherical bubbles continue to grow by normal loop-punching.

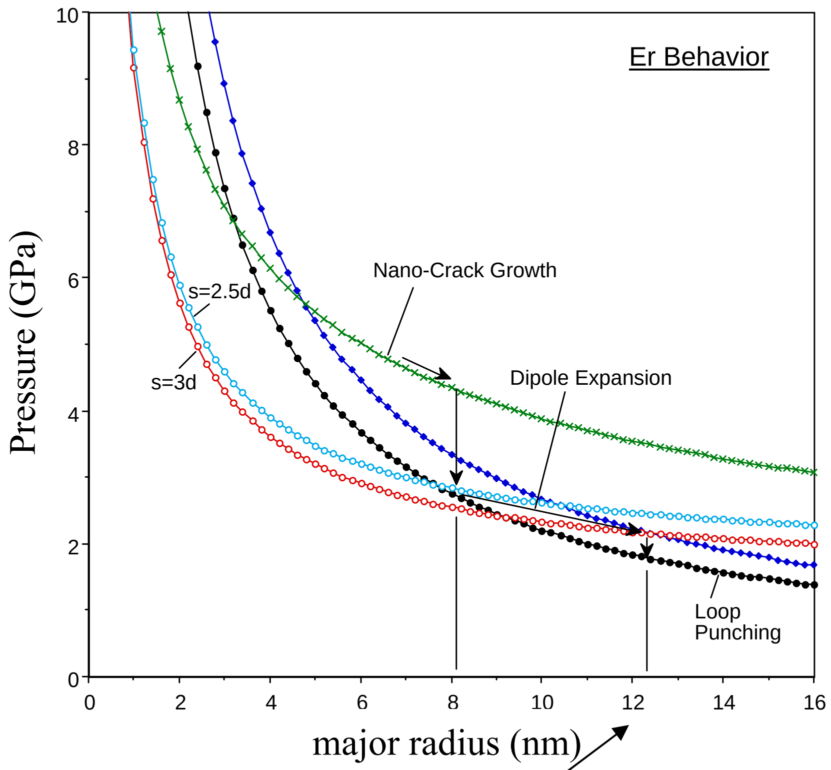


Lattice dilation “details” of PdT appear to support the existence of multiple stages.

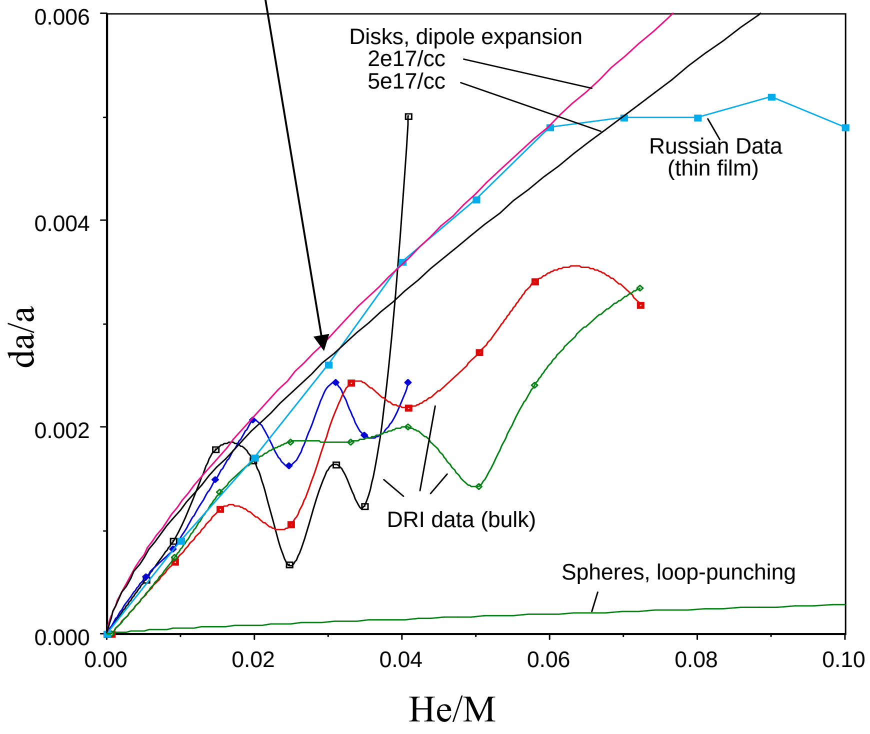


- Initial Griffith crack growth at high pressure will produce an even rise.
- The bubble volume increases by 8X during the transition from platelets to spheres.
- Emitted dislocations must remain trapped between “bubbles”.
  - Bubble source volumes remain constant!)

The He precipitates in Er tritide remain 2-dimensional throughout life.



- Pressure changes during transions from nano-cracks to platelets may explain oscillations in bulk da/a data.



- The linking of large platelets by should begin prior to the spherical transition, where ΔA/A≈3.

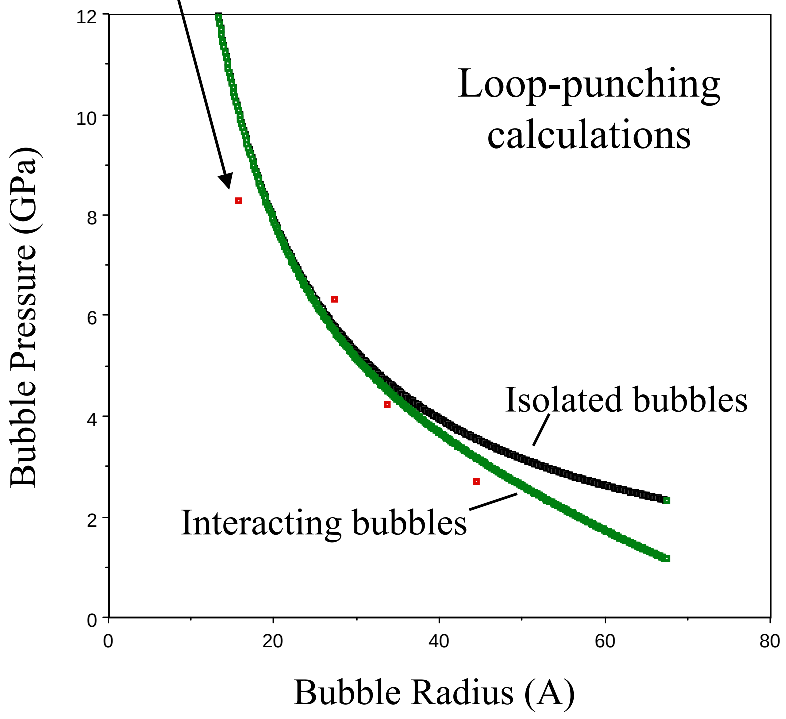
Work on platelet structures is continuing.

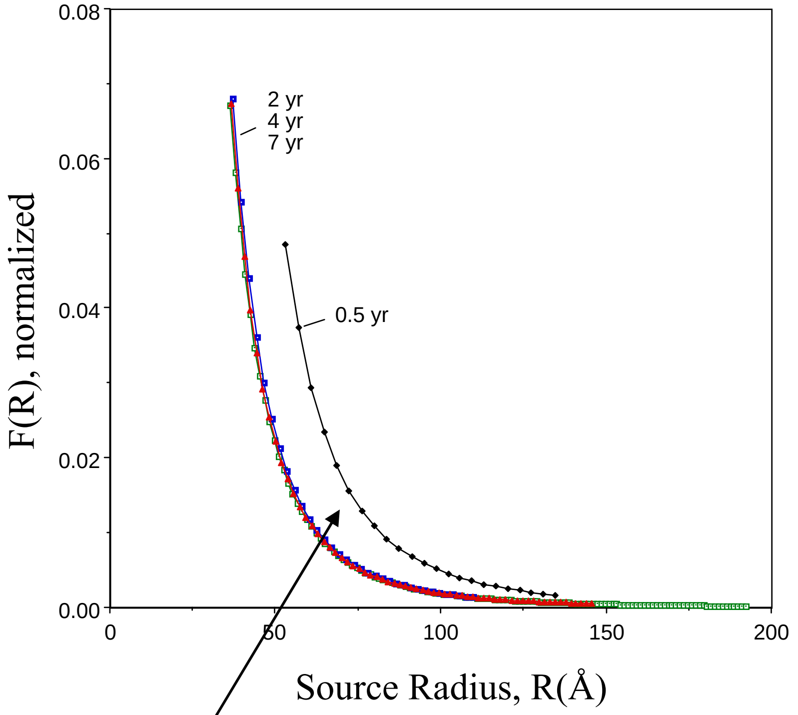
- Thin (111) platelet bubbles can be associated with nano-cracks or dislocation dipole structures.
- Additional theoretical work is examining
  - formulations of platelet characteristics
  - linking of platelets by inter-platelet fracture
- Continued testing will examine
  - the bubble pressure and spacing distribution from 6 month-old Pd tritide (in spherical transion stage).
  - observed bubble shapes in other materials (e.g. SiC).
  - observed bubble shapes in implanted materials.
  - early decrease of Pd tritide plateau pressure (better data needed).
  - proposed TEM studies in selected materials to characterize shapes and identify transition points.
- A comprehensive effort to obtain model-testing data should improve early bubble characterization in PdT.

The bubble pressure and spacing distribution for young PdT deviate from spherical growth.

- A platelet shape will lower the computed bubble pressure at 0.5 yr
  - from 10 to 8 GPa,

  and produce better agreement with the pressure deduced by NMR.





- It will also change the bubble spacing distribution computed for the 0.5 yr sample.

Technique	Information	Existing Pd Data (agree, disagree)
TEM: Brewer, Gelles (PNNL)	He bubbles Number density, size, distributions Profiles, effect of intrinsic defects on nucl. Onset of *IB-fracture, μ-fracture network percol.*	n_B - Thomas, n_B - Thiebaut r(He/M) - Thiebaut
NMR: Curro (LANL), Cowgill	He atoms in bubbles He density distrib. (& pressure from EOS) Changes with temp, anneal, phase *Effect of bubble interactions / IB-fracture*	v_{He}(dist, He/M) - Abell $\Delta v_{He}/\Delta\Phi$ - Cowgill
Swelling:	Integrated bubble volume, ΔT & $\Delta\Phi$ effects (Onset of IB-fracture?)	$\Delta V/V$(He/M) - Guthrie, Abell
XRD, PCT: Majzoub, Walters (SRNL)	Lattice strain, mean bubble press., ΔT effects PCT shifts (plateau, boundaries)	da/a - Thiebaut Δp_H - Guthrie
Early He Release (ERF): Cowgill, Mintz (LLNL)	He escape depth, bubble profile *Dependence on nucleation conditions*	ERF - Meyer
He Thermodesorption: Walters (SRNL)	*μ-fracture network percolation* *Effects of powder particle size*	Crit. He/M - Coronado, Meyer
He-Implanted Material: Hertz	TEM, NMR, swelling for growth & fracture data; XRD for lattice strain; n-indent for E*	$\Delta V/V$(He/M) - Pontau, Hertz n_B - Gelles
Nano-indentation: Moody, Knapp	Mechanical props. of un-aged & aged material Elastic modulus of composite	$c_{ij}(t_o)$ - (Wolfer), $c_{ij}(t)$ - Schwarz $E^*(t_o)$ - Fabre
He Implant/Re-emission: Cowgill	He diffusivity, pairing energy Temperature dependences	D_{He} - Cowgill
SAXS/SANS/PAS/EXAFS/EELS: Majzoub, Browning, Hertz	Bubble data? (Onset of bubble coalescence / IB-fracture?)	R(EXAFS) - Thiebaut