Phase-Field Theory of Amorphous Nano-Phases

Alex Umantsev

Fayetteville State University,
Fayetteville, NC

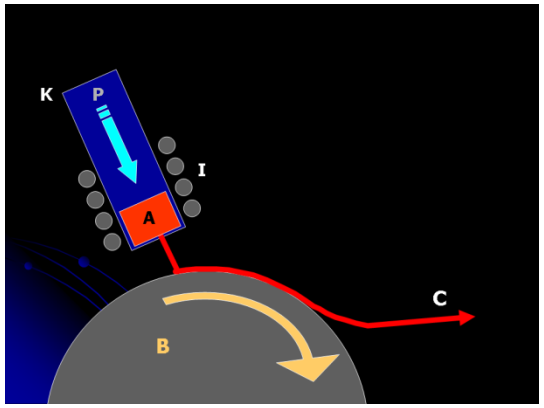
CHiMaD

National Science Foundation
WHERE DISCOVERIES BEGIN

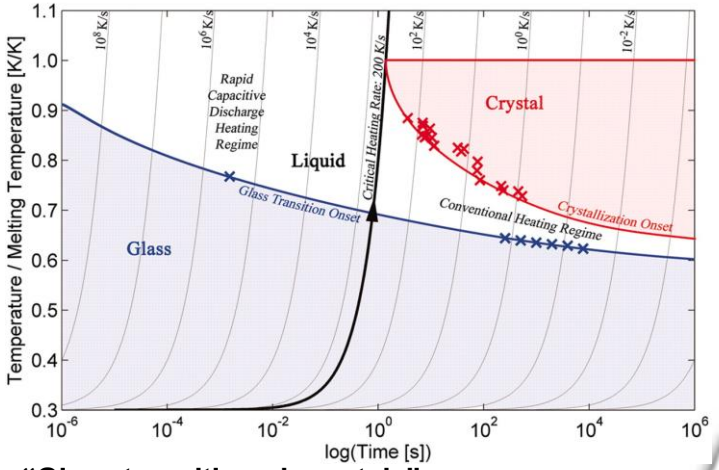
Outline

- What this presentation is NOT about
- Experiments
- Theory
- Generalization (if time allows)

Amorphous Bulk Materials—Glasses



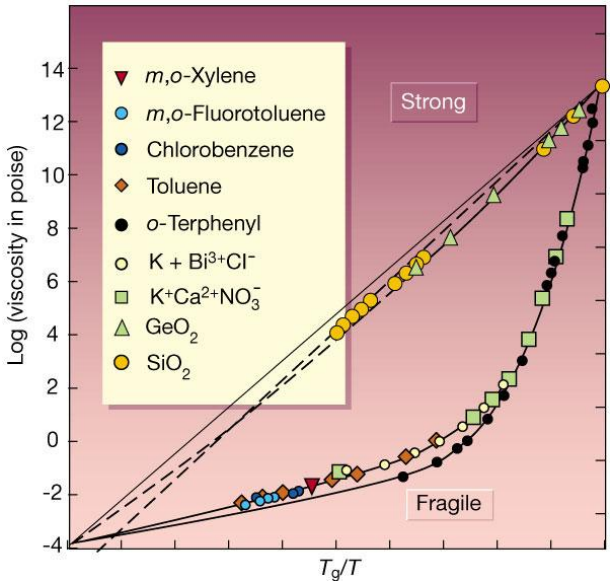
"Melt spinning process" Wikipedia



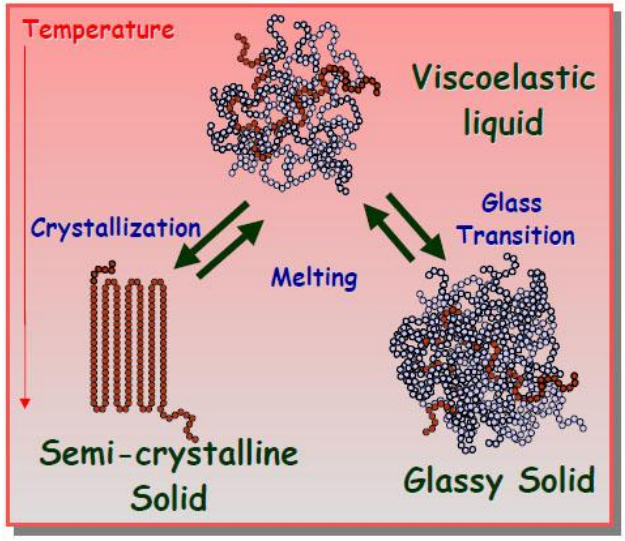
"Glass transitions in metals"
W L Johnson et al. Science 2011;332:828-833

This presentation is NOT about glasses.

Your local Sporting Goods store



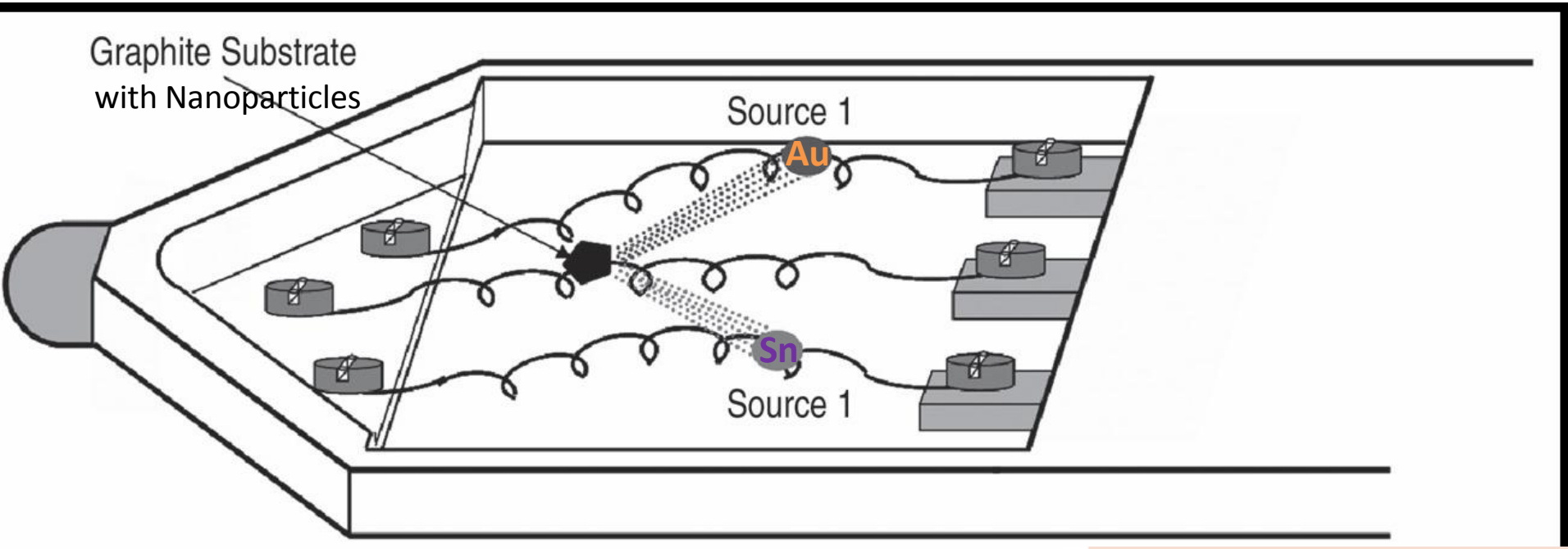
Angell et al



Geotechnical Engineers

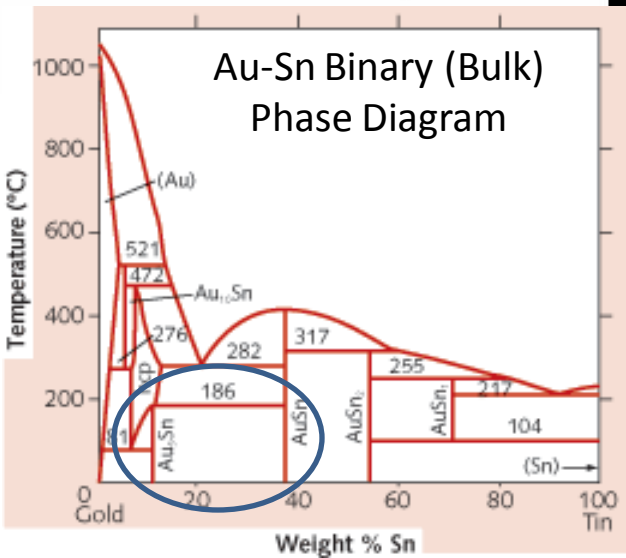
Double-Source Evaporator

H. Yasuda and H. Mori, Osaka University, Japan



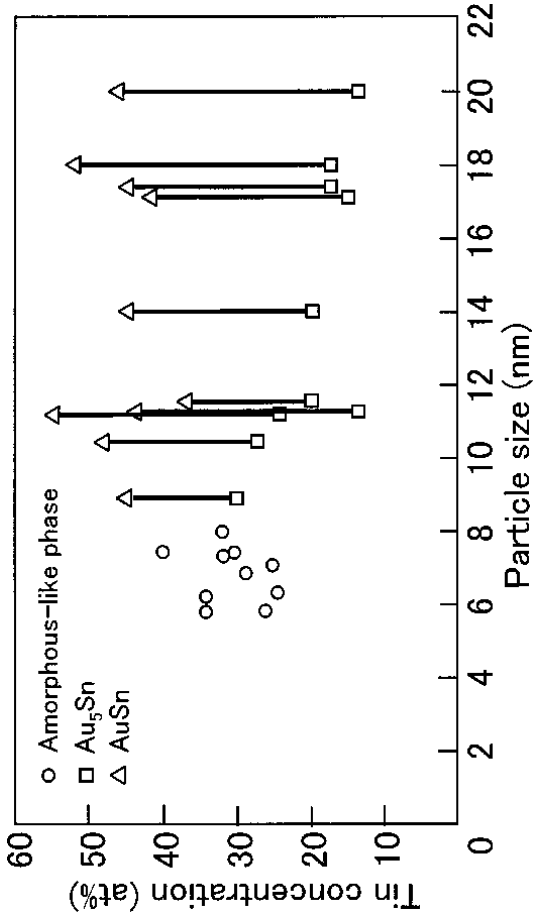
In situ TEM

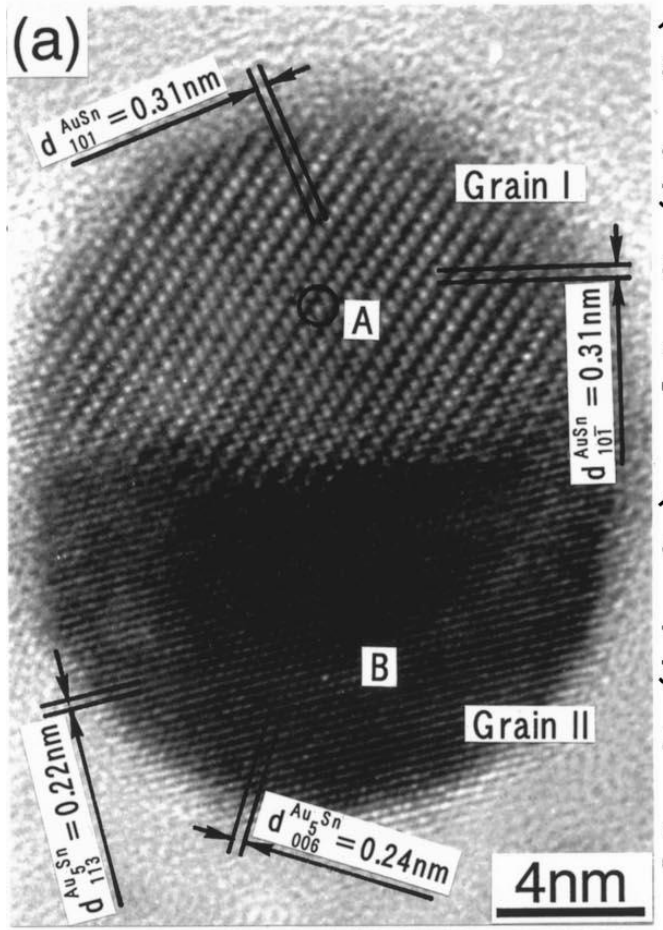
Hot, dry metallurgy

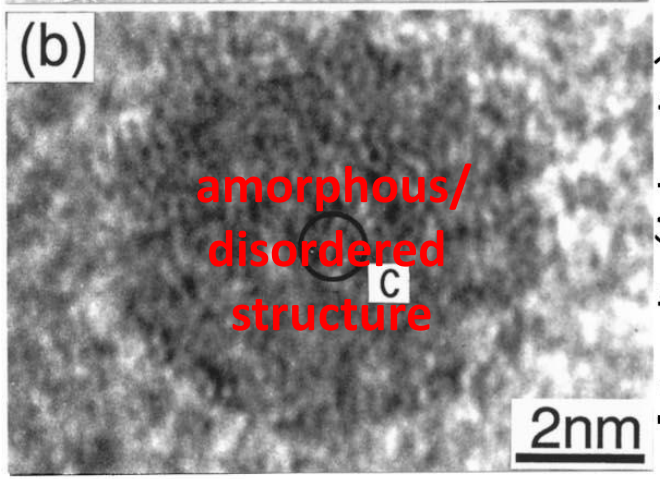


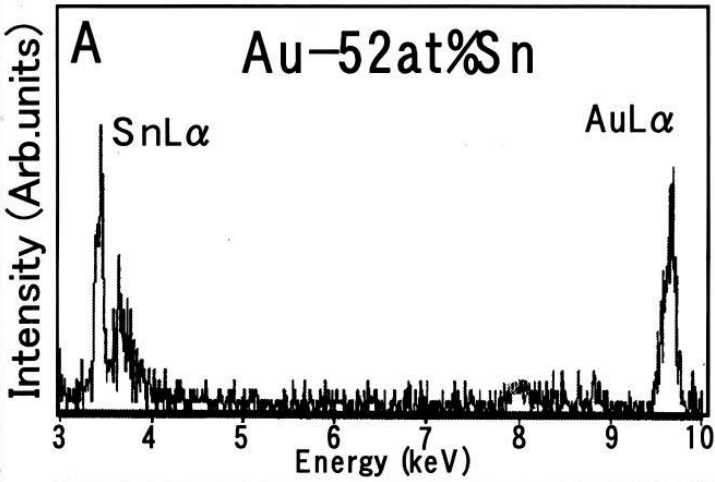
Binary systems: Sn-Au-(Sb, Bi, In, Pb, Zn, Cu)

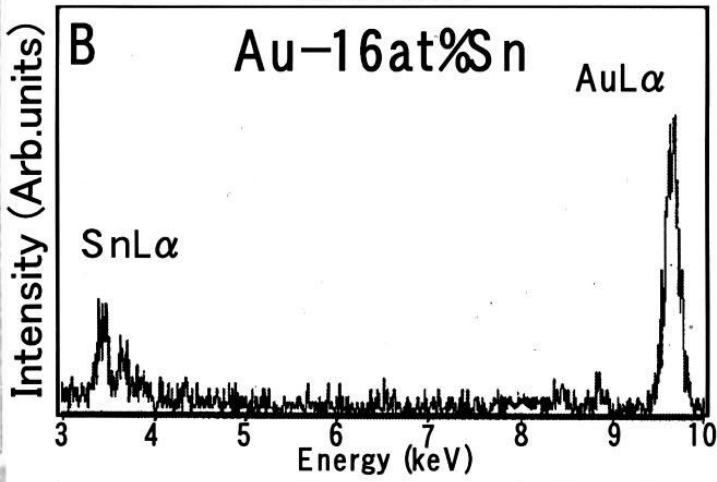
Ternary system: Sn-Au-Pb ~1991-2006

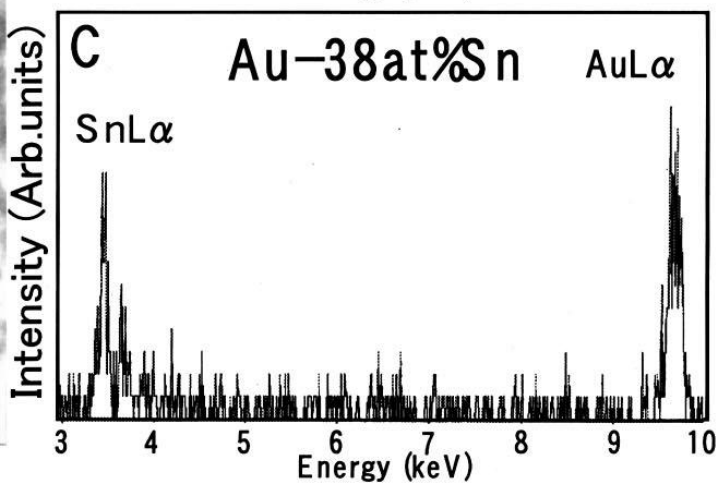

Tin concentration (at%)
60
50
40
30
20
10
0
Particle size (nm)
0
2
4
6
8
10
12
14
16
18
20
22
Amorphous-like phase
Au5Sn
AuSn

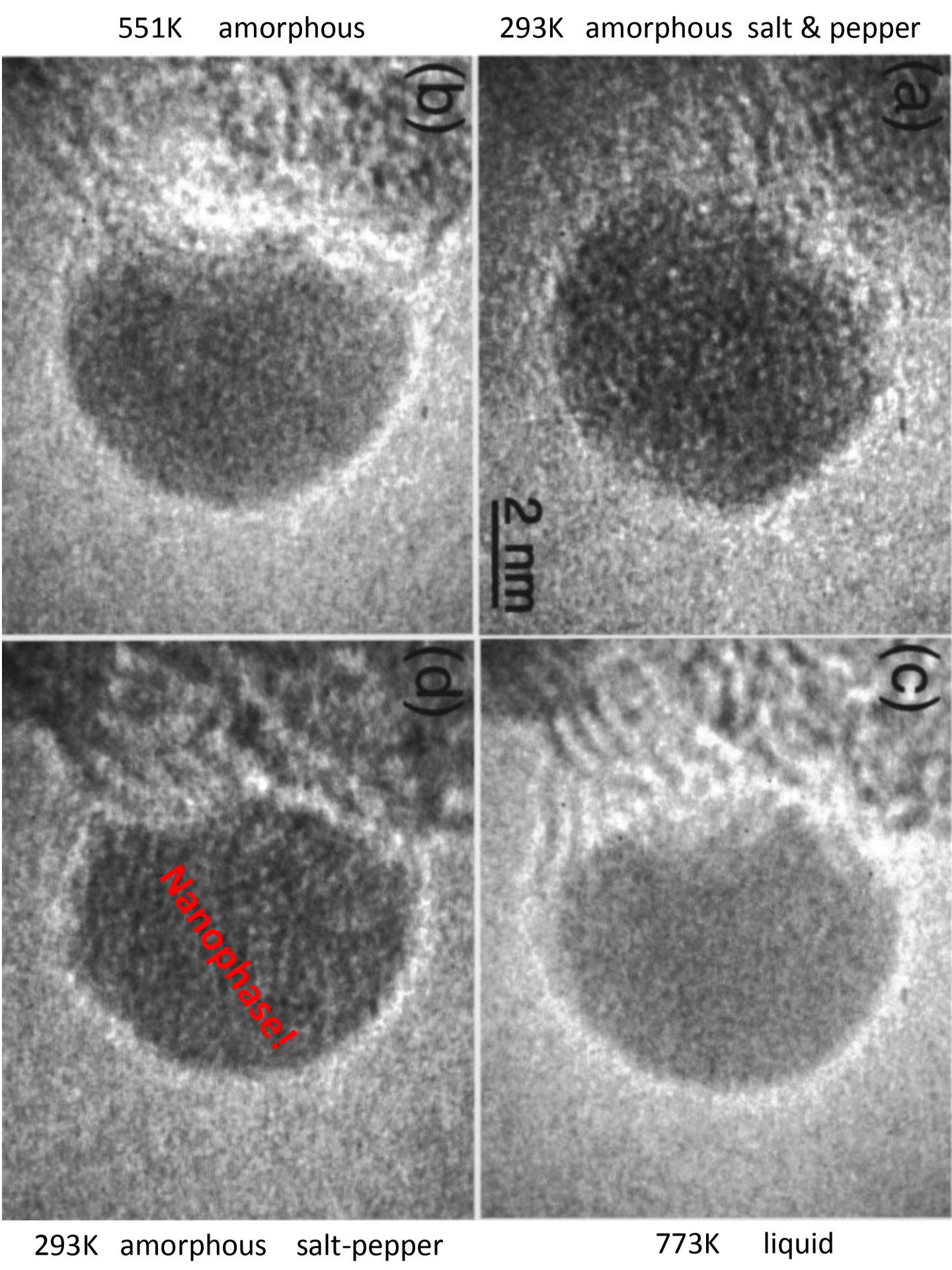

(a)
d AuSn 101 = 0.31nm
Grain I
A
d AuSn 10T = 0.31nm
B
Grain II
d Au5Sn 113 = 0.22nm
d Au5Sn 006 = 0.24nm
4nm


(b)
amorphous/
disordered
structure
C
2nm


A
Au–52at%Sn
SnLα
AuLα
Intensity (Arb.units)
3
4
5
6
7
8
9
10
Energy (keV)


B
Au–16at%Sn
AuLα
SnLα
Intensity (Arb.units)
3
4
5
6
7
8
9
10
Energy (keV)

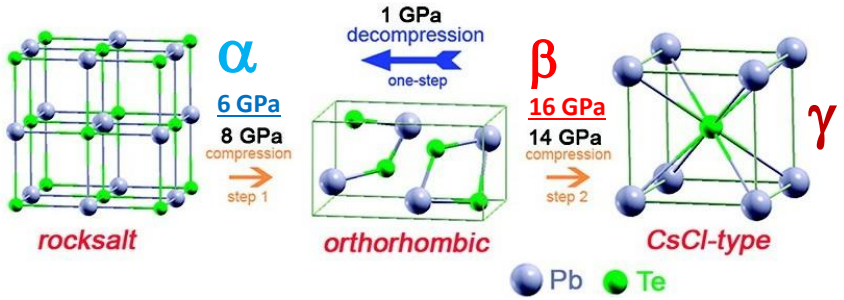

C
Au–38at%Sn
AuLα
SnLα
Intensity (Arb.units)
3
4
5
6
7
8
9
10
Energy (keV)

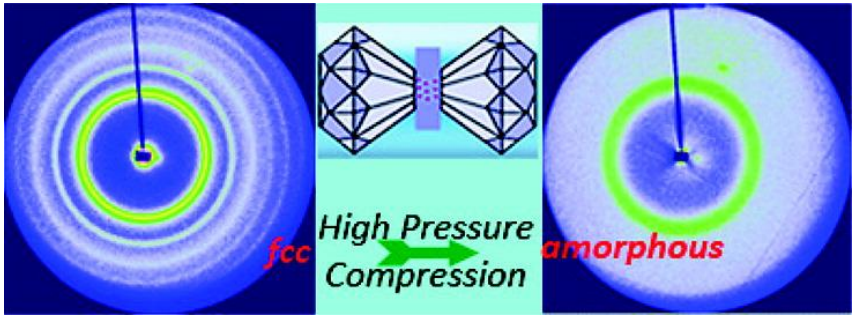

551K amorphous
293K amorphous salt & pepper
(b)
(a)
2 nm
(d)
(c)
Nanophase!
293K amorphous salt-pepper
773K liquid

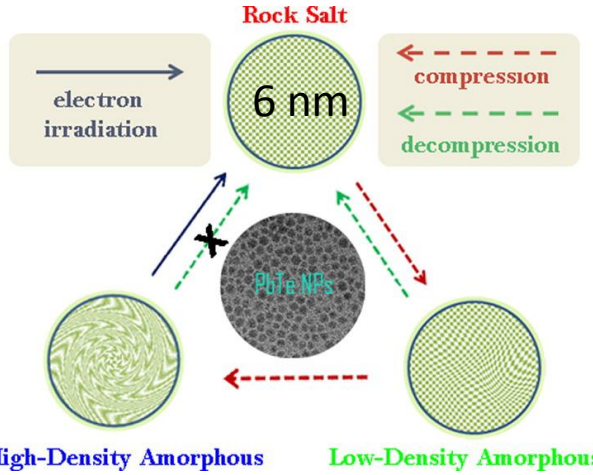
High-Pressure Transformations in Lead-Telluride Nano-Particles

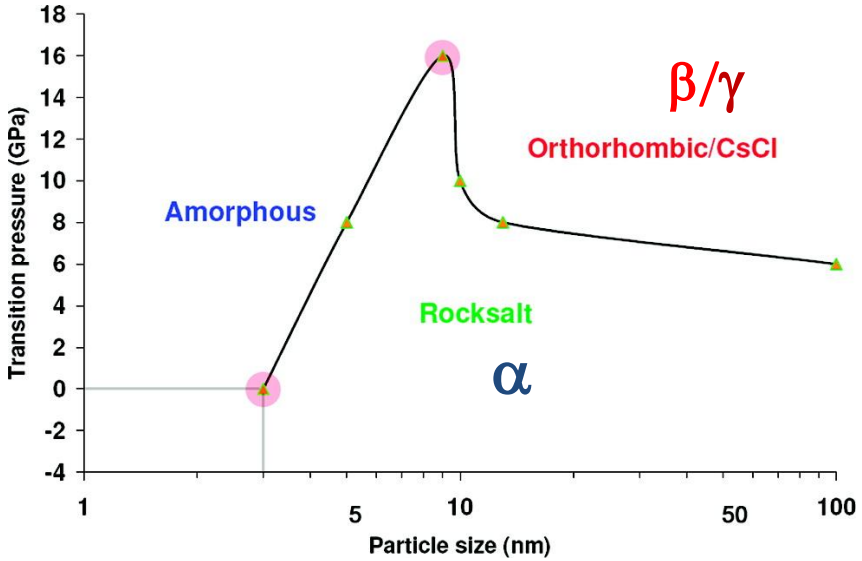
J. Fang et al, NANOLetters '11, '13

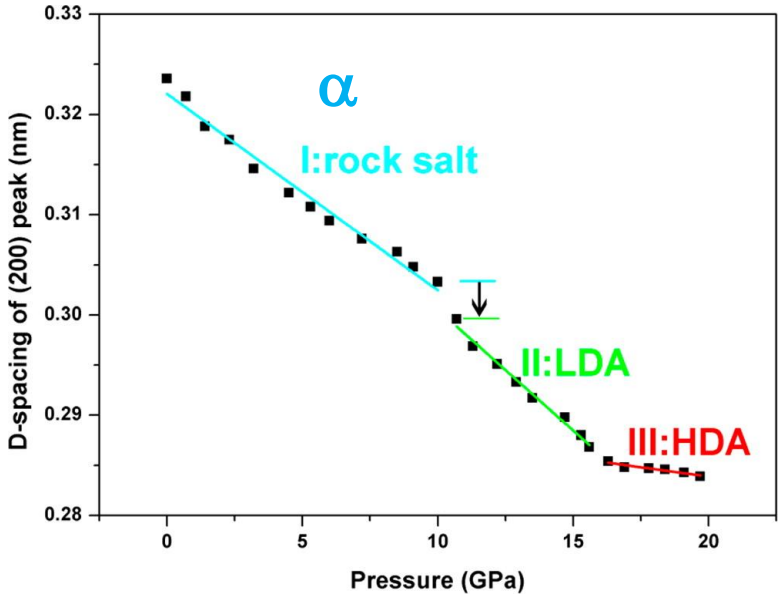
Bulk Phase Diagram











Amorphization of Elemental Metals

Acta metall. Vol. 36, No. 9, pp. 2525–2536, 1988
Printed in Great Britain.

0001-6160/88 $3.00 + 0.00

SOLIDIFICATION STRUCTURES IN SUBMICRON SPHERES OF IRON–NICKEL: EXPERIMENTAL OBSERVATIONS†

YEON-WOOK KIM, HONG-MING LIN and THOMAS F. KELLY
Department of Metallurgical and Mineral Engineering, University of Wisconsin, Madison, WI 53706, U.S.A.

(*Received* 17 *June* 1987; *in revised form* 9 *December* 1987)

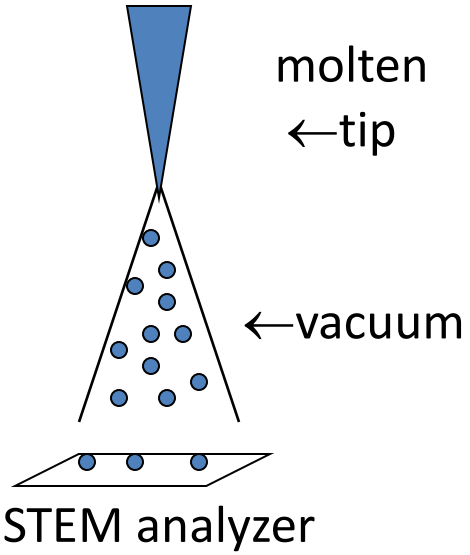
Acta metall. Vol. 37, No. 1, pp. 247–255, 1989
Printed in Great Britain.

0001-6160/89 $3.00 + 0.00

AMORPHOUS SOLIDIFICATION OF PURE METALS IN SUBMICRON SPHERES†

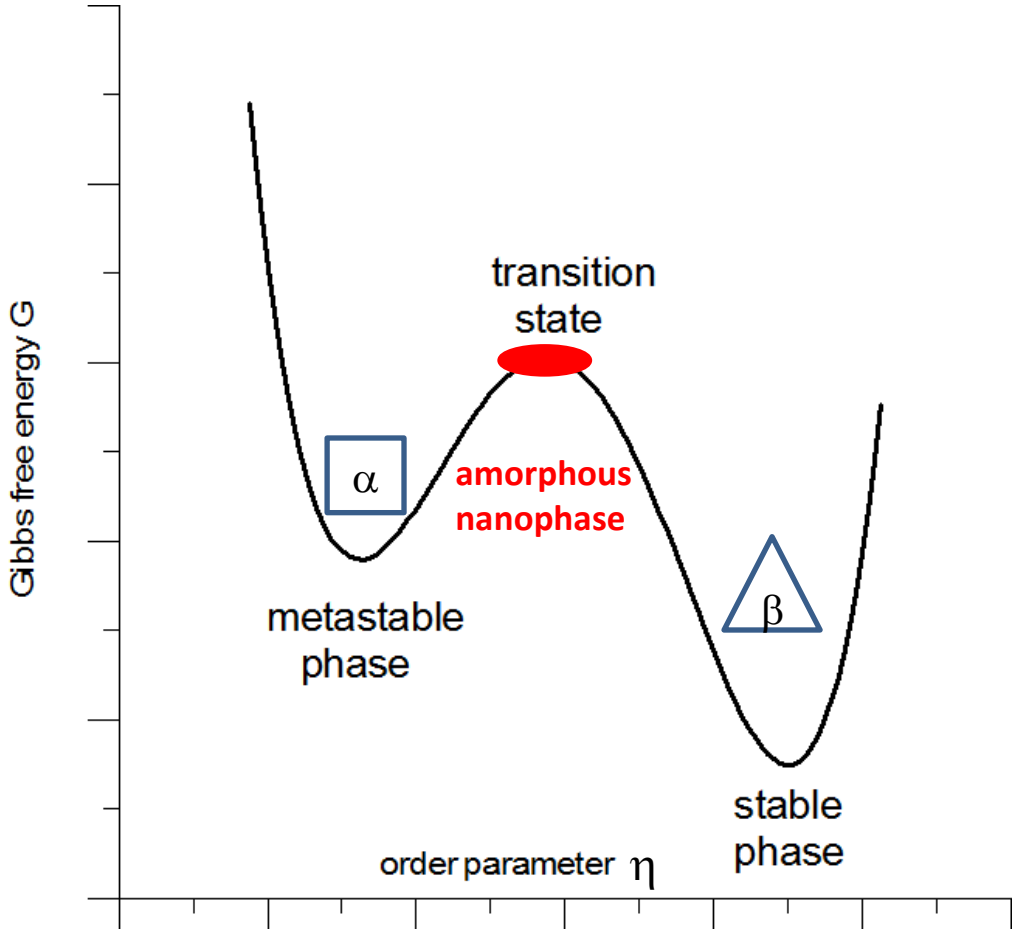
YEON-WOOK KIM, HONG-MING LIN and T. F. KELLY
Department of Metallurgical and Mineral Engineering, University of Wisconsin—Madison, Madison, WI 53706, U.S.A.

(*Received* 9 *March* 1988)



Nanoparticles of 15 elemental metals plus silicon and germanium sprayed in vacuum solidify into **amorphous phase.**

Phase-Field Explanation



What is the nature of the amorphous phase?

What is the relation between the amorphous phase and the bulk phases?

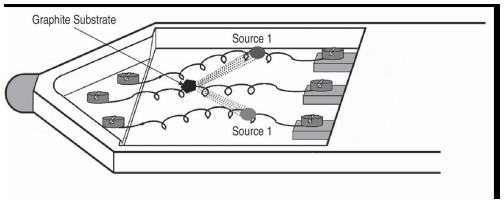
No explanation!

Two-Phase Closed-System Thermodynamics

$$4\,U_2[X_2]^2 > W = 24\,V_m\frac{\sigma}{l}$$

σ --Interface energy

l --Interface thickness

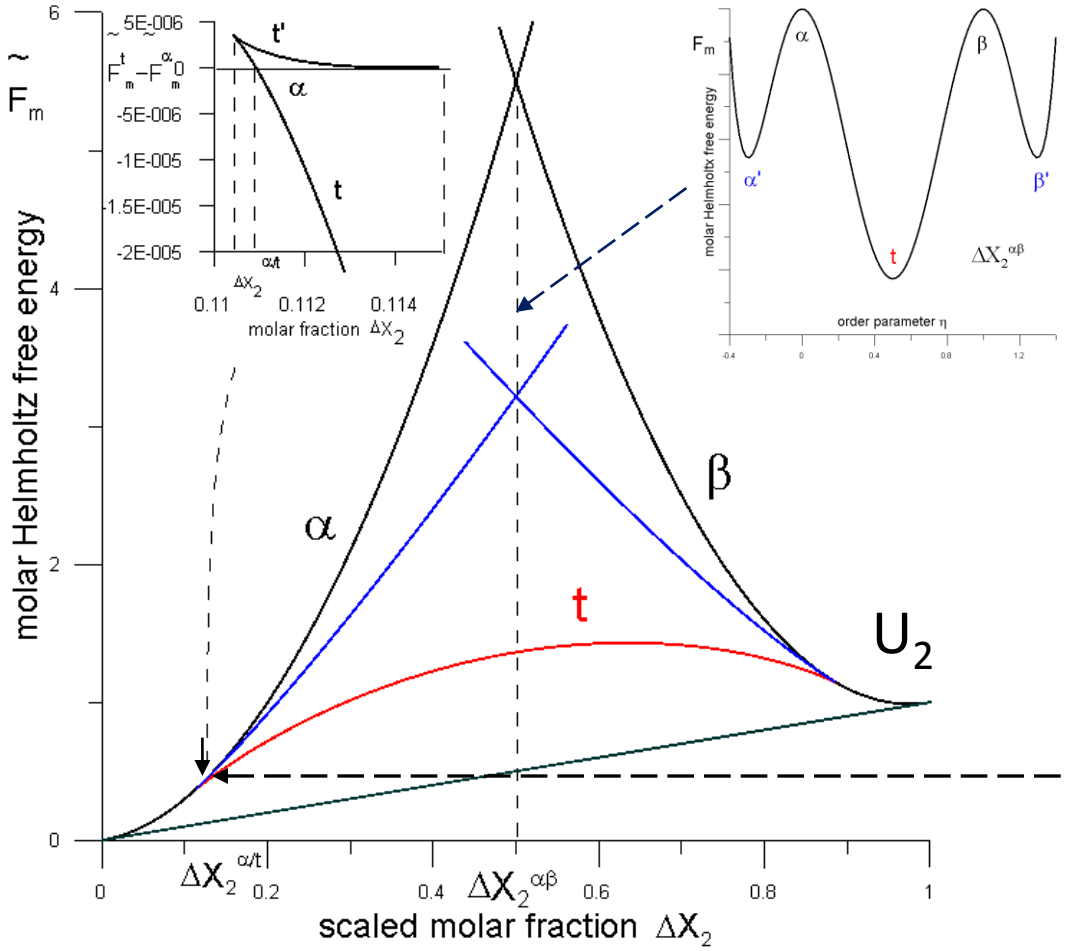


Two Constrains:

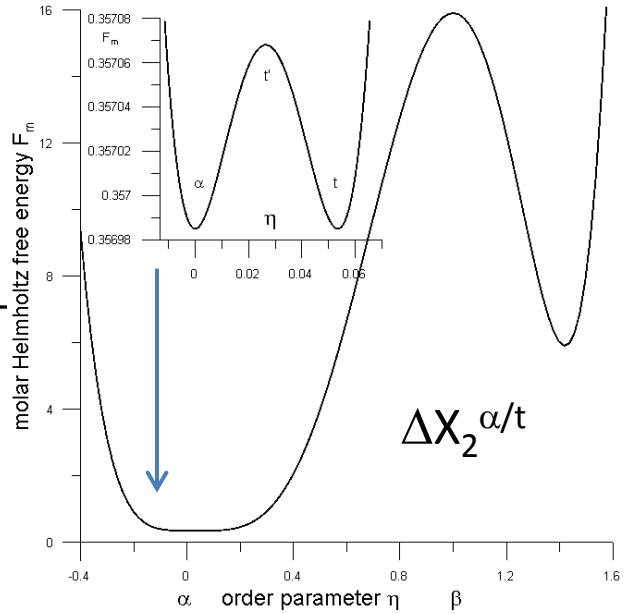
1) Closed system
2) Small system

Two Criteria

1) Material parameters criterion
2) Specific range of compositions



First-order close to second-order



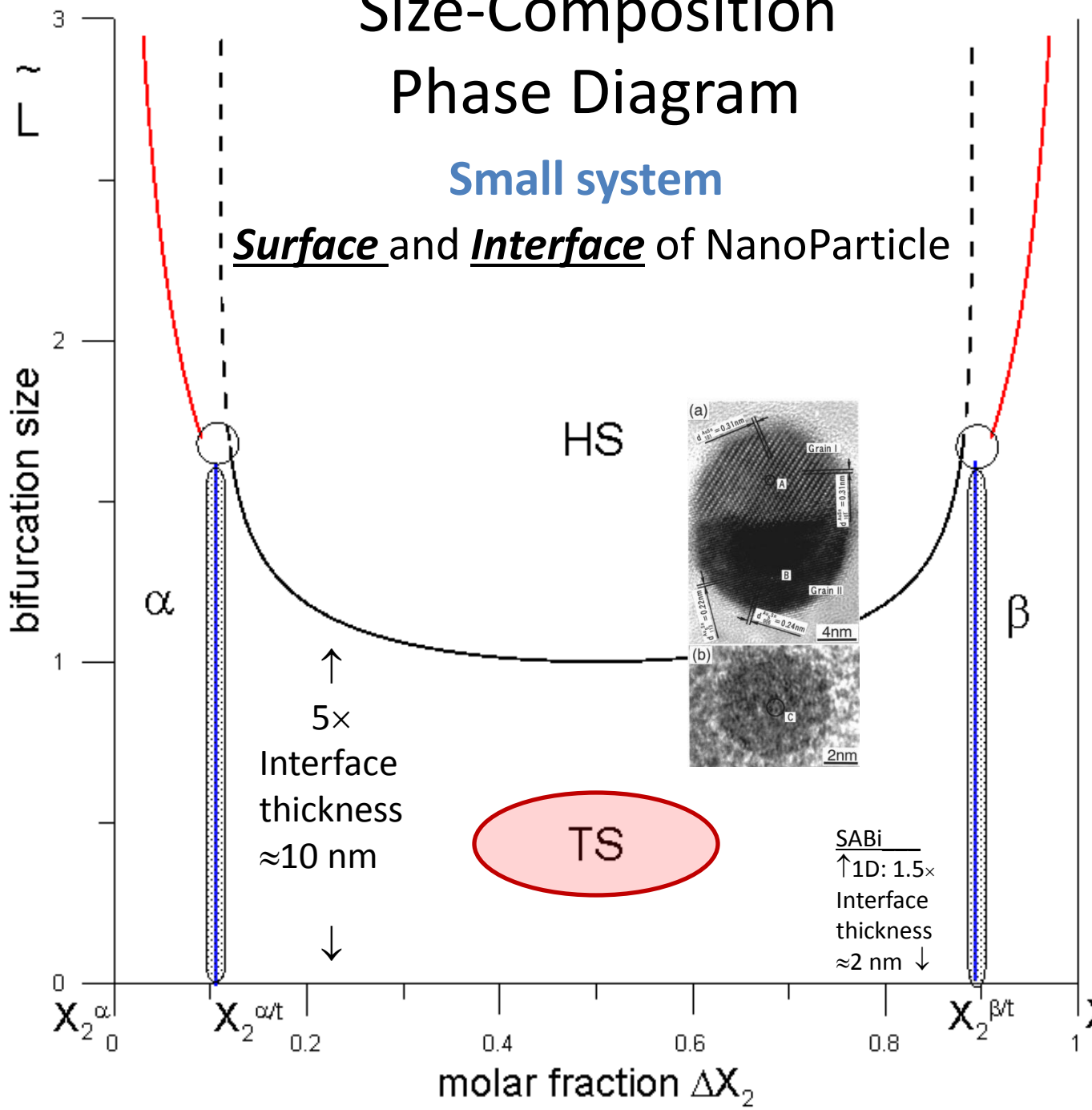
← $[X_2]$ →

Acta Materialia **61**, 1106-1117 (2013)

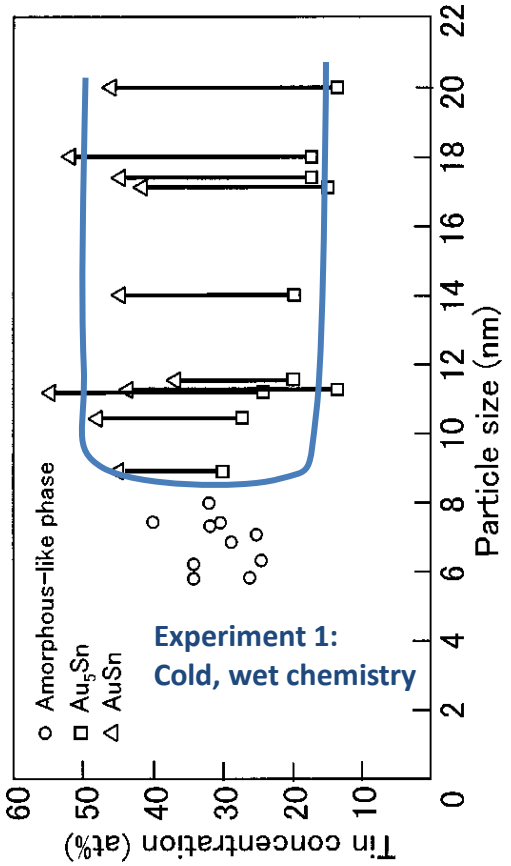
Size-Composition Phase Diagram

Small system

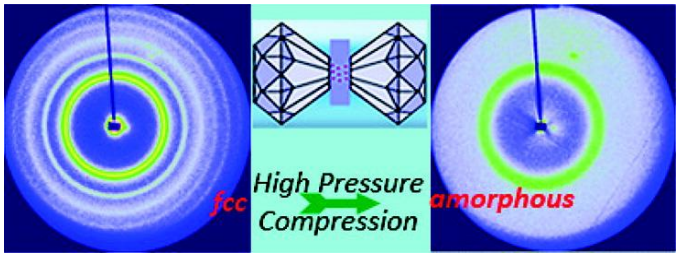
Surface and ***Interface*** of NanoParticle

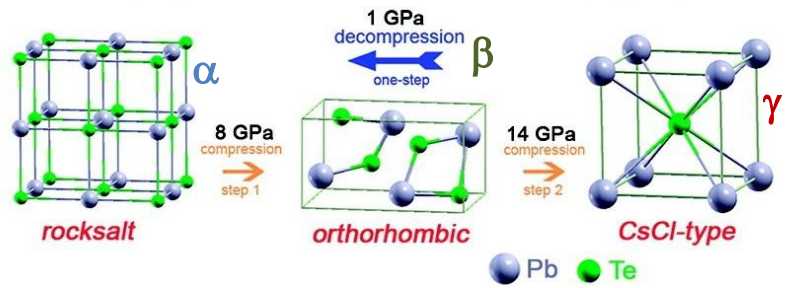


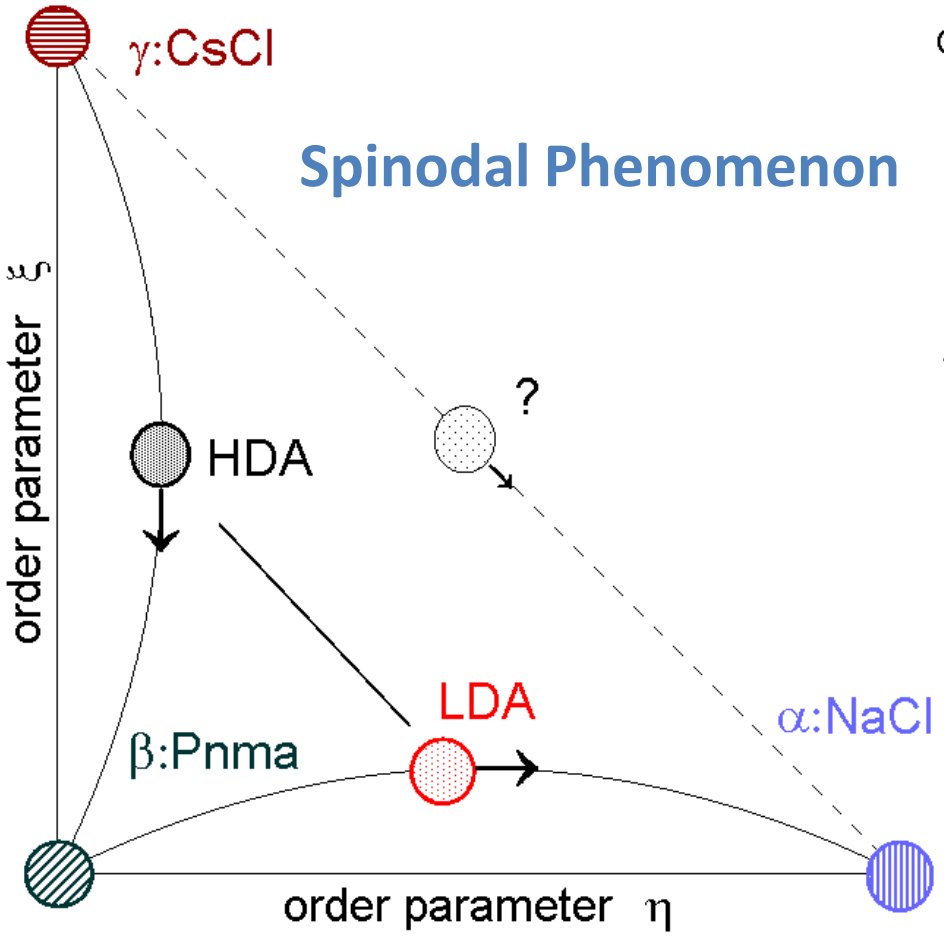
Experiment 2: Expose the NanoParticles to the wind of tin or gold atoms. Prediction: NP should transform to the respective intermetallic phase



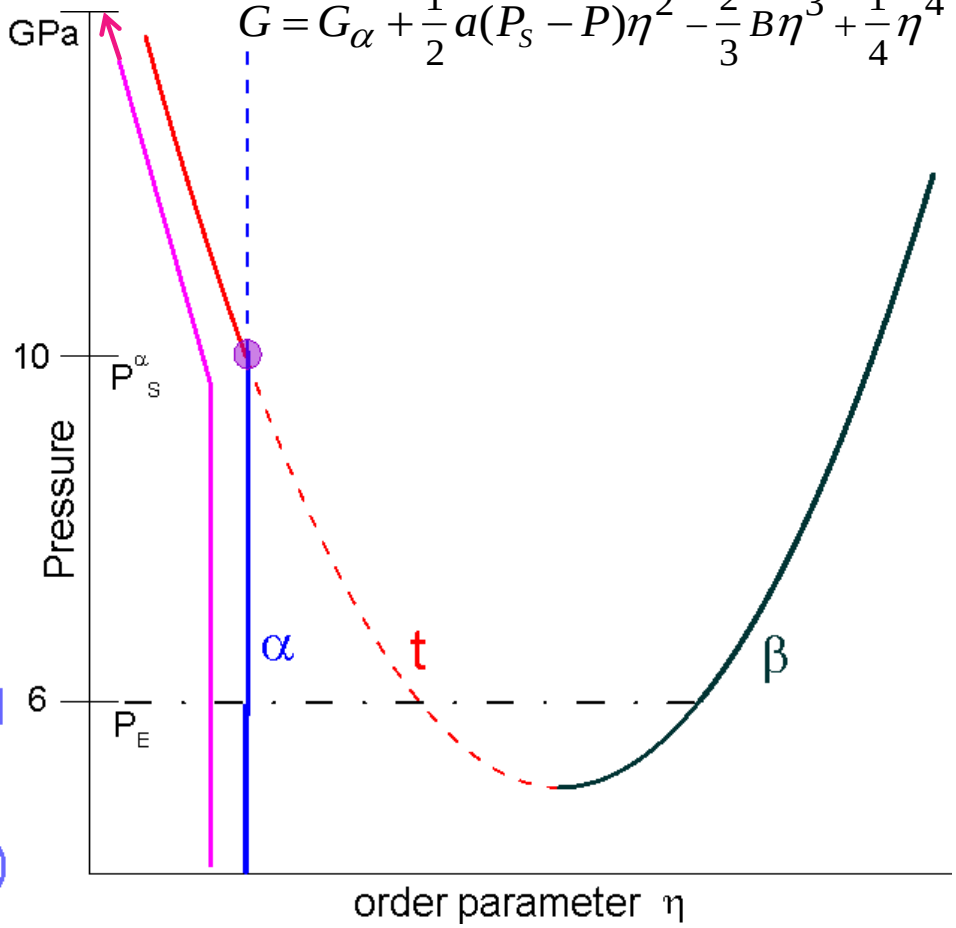
High-Pressure Transformation in Pb-Te NPs



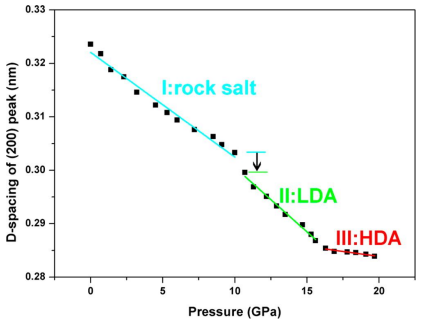


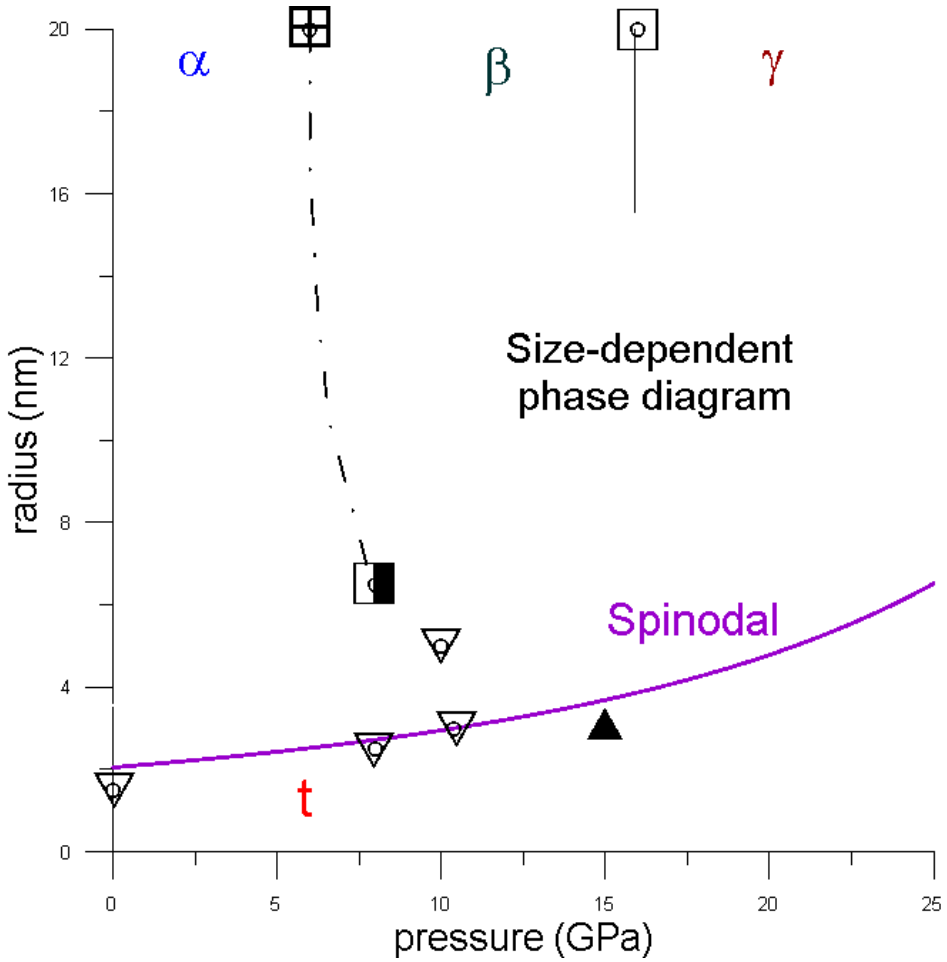


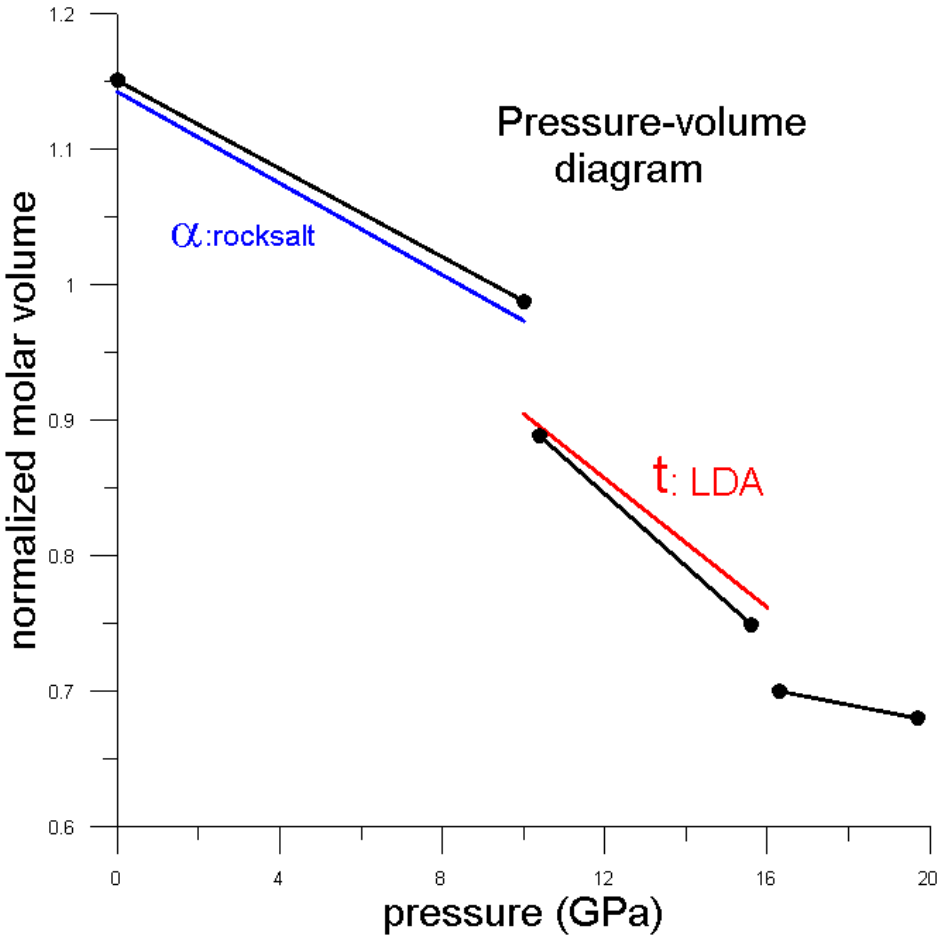
$$G = G_\alpha + \frac{1}{2}a(P_S - P)\eta^2 - \frac{2}{3}B\eta^3 + \frac{1}{4}\eta^4$$



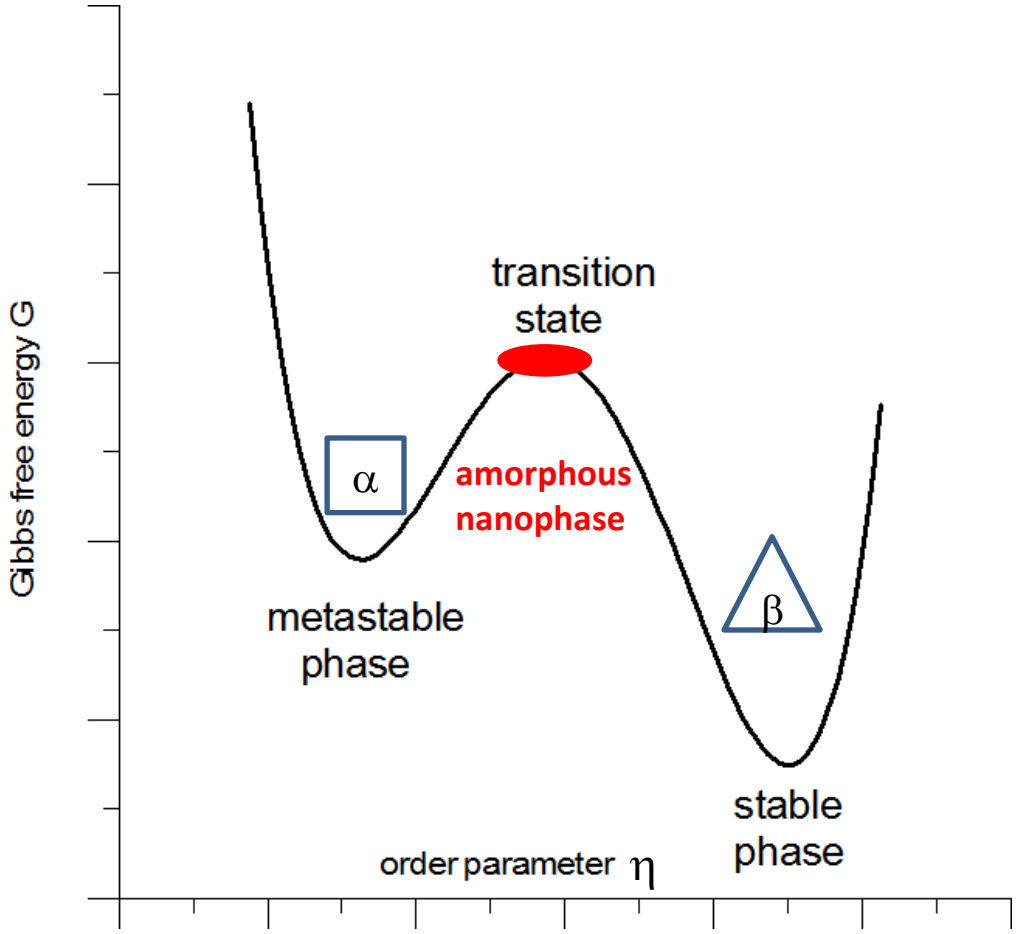
High-Pressure Transformation in Pb-Te NPs



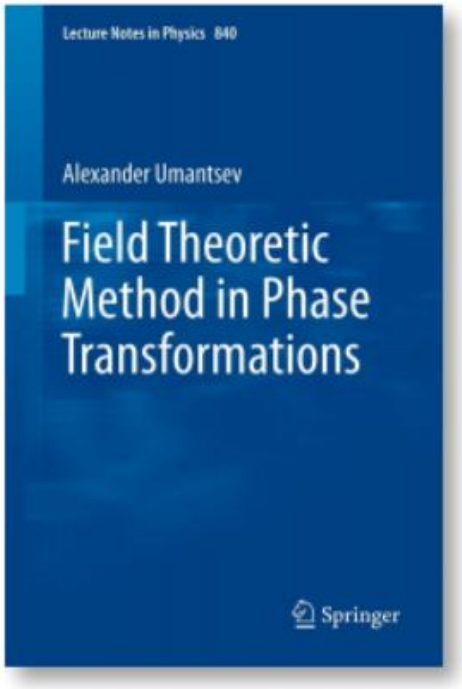




Conclusion



The explanation that the amorphous nanophases is represented by the transition state of the free energy works!



2012, X, 344 p. 55 illus., 27 illus. in color.

A. Umantsev

Field Theoretic Method in Phase Transformations

Series: Lecture Notes in Physics, Vol. 840

- Describes the novel and very popular method of theoretical and computational study of phase transformations and materials processing in condensed and soft matter
- Discusses the foundations of the method along with the advanced results in a single volume
- Serves as a primer in the area of phase transformations and as a guide for a seasoned researcher

The continuum, field theoretic method of study of phase transformations in material systems, also known as "phase field", allows one to analyze different stages of transformations on the unified platform. It has received significant attention in the materials science community recently due to many successes in solving or illuminating important problems. This book will address fundamentals of the method starting from the classical theories of phase transitions, the most important theoretical and computational results, and some of the most advanced recent applications.

Field Theoretic Method in Phase Transformations can be used as an introduction for those new to the field or as a guide for a seasoned researcher. It is also of interest to researchers interested in the history of physics.