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Effect of nucleation on the stability of *BCC* In-Tl alloy

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Abstract : *BCC* In-Tl alloy is chosen to study the effect of nucleation on its mechanical stability in the framework of extended generalised exponential potential by employing Born stability criteria, which eventually leads to a phase transition from body-centered cubic (*bcc*) to body-centered tetragonal (*bct*) structure. The general procedure presented is independent of the specific model of interatomic interactions which may be used in numerical calculations. In the present study, a detailed numerical calculations are undertaken to compute the theoretical strength and range of stability of a perfect uniaxially (100) stressed crystal lattice of *bcc* In-Tl alloy under homogeneous tension and compression. The study reveals that *bcc* In-Tl alloy is composed of two ranges of stability—one for body-centered cubic (*bcc*) phase and another for body-centered-tetragonal (*bct*) phase At each stage of deformation, the second-order elastic constants C_{11} and C_{12} are calculated. Although no specific experimental results related to present study of strength and stability of *bcc* In-Tl alloy are available in the literature, the computed values of theoretical strength and strain of the alloy of present concern, lies well within the general experimental limits.

Keywords : Nucleation, Born stability criteria, In-Tl alloy

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1. Introduction

The concept of nucleation is intimately related with the structural phase transition in the crystalline solids. In fact, phase transitions in any system are caused by inducing nucleation in its structure, by arbitrary homogeneous deformations under the application of external

forces. The study is of interest because the values of stress and strain at which the crystalline solid becomes mechanically unstable in terms of Born criteria [1] represents the theoretical strength of the crystalline solid and hence an upper limit to the actual strength of the solids.

Nucleation basically refers to directional non-identity of ionic separations, which eventually alters the range of intervening forces under uniform deformations and results into a change in the lattice structure, applied stress, internal energy and elastic constants of the crystalline solid under consideration. The continued application of nucleation to a system helps us to know the quantum of external force which the system can bear safely and hence acts as a useful guide to check the stability of the material in question. The deformations usually referred as twinning or nucleation [2] leading to structural transition from tetragonal to orthorhombic phase have a direct bearing on the process of hot superconductors [3]. The orthorhombic phase nucleates [4] along the grain boundaries and then propagates into the interiers of the grains, which are initially tetragonal and hence non-superconducting. The elastic properties of superconductors are also considerably affected [5] on account of nucleation resulting into phase transition from tetragonal to orthorhombic structure. The present study, however deals with the problem of theoretical strength and stability of *bcc* In-Tl alloy under nucleation from cubic to tetragonal phase.

An alloy is composed of its metallic constituents and the response of its metallic constituents *i.e.* ions and electrons subjected to the process of nucleation may be partly linear and partly non-linear. The nature of electron behaviour calls for the inclusion of anharmonic non-linear interactions in the alloy. The process of nucleation of cubic structure, essentially invoking phase transitions, necessitates coherent changes in range, strength, and nature of intervening bindings. An effective and appropriate potential embodying the required non-linearity and desired width and depth is needed to explain nucleation in *bcc* In-Tl alloy.

The previously developed extended generalised exponential potential (EGEP), being amply capable of explaining static [6] and dynamic [7] behaviour of cubic metals, is further employed to explain the elastic behaviour of simple *bcc* structures subjected to the process of nucleation [8,9].

2. Theory

2.1. Extended generalised exponential potential :

The attractive as well as the repulsive components of the generalised exponential potential [10] have been extended for representing their true and realistic nature. Extended generalised form of exponential potential (EGEP) so developed assumes the form

$$\Phi_m(r_{ij}) = D/(m-1)\left[e^{-m\alpha(r_{ij}-r_0)}/(\alpha r_{ij})^n - m(\alpha r_{ij})^n\, e^{-\alpha(r_{ij}-r_0)}\right]. \qquad (1)$$

The average interaction (cohesive energy) energy per atom within the framework of EGEP is

$$\Phi_m(r) = D/2(m-1) \sum_j \left[e^{-m\alpha(r_j - r_0)}/(\alpha r_j)^n - m(\alpha r_j)^n e^{-\alpha(r_j - r_0)} \right]. \quad (2)$$

where m and n are the parameters which takes care of electronic exchange and correlation effects and three-body forces such as volume forces in an alternative and simpler form respectively, D is the dissociation energy, α the hardness parameter and r_0 the equilibrium separation parameter.

The details concerning the evaluation of the parameters of the potential are mentioned in our recent earlier paper [7]. The input data for *bcc* In-Tl alloy studied and its computed potential parameters are given in Tables 1 and 2 respectively.

2.2. Theoretical considerations :

The necessary and sufficient conditions [11] for a lattice to be in stable equilibrium under the effect of uniaxial stress in [100] direction in terms of Born stability criteria takes the form

$$B_{11} > 0, \quad B_{22} > 0, \quad B_{12} > 0, \quad B_{23} > 0, \quad (3)$$

$$AA = B_{22} - B_{23} > 0, \quad (4)$$

$$BB = B_{11}(B_{22} + B_{23}) - 2(B_{12})^2 > 0, \quad (5)$$

where $$B_{ij} = \left[\frac{\partial^2 E}{\partial a_i \, \partial a_j} \right] \quad (6)$$

and E is the energy per unit cell given by

$$E = (1/2)\, n' \sum_{l_1 l_2 l_3} \phi(r). \quad (7)$$

i and j have their values ranging from 1 to 6 and n' is the number of atoms per unit cell. The parameters a_1, a_2 and a_3 stand for semi-lattice constants along the three edges of the unit cell of the cube and a_4, a_5 and a_6 are the angles between a_2 and a_3, a_3 and a_1, a_1 and a_2 respectively. The normal stress acting on a face of the unit cell, when the cell edges are perpendicular to each other is given by

$$= \frac{1}{a_2 a_3} \left[\frac{\partial E}{\partial a_1} \right]. \quad (8)$$

The force F_1 acting on the crystal lattice in the direction a_1 is given by (*i.e.* uniaxial [100] expansion or contraction)

$$F_1 = \left[\frac{\partial E}{\partial a_1} \right] \quad (9)$$

and the force F_2 acting along a_2 is

$$F_2 = \left[\frac{\partial E}{\partial a_2}\right] = 0, \tag{10}$$

where for a tetragonal crystal lattice

$$a_2 = a_3 \quad \text{and} \quad a_4 = a_5 = a_6 = \pi/2. \tag{11}$$

The modulii B_{ij} embodied in eqs. (3) to (5) are given by (with $n' = 2$ for *bcc* lattice)

$$B_{11} = a_1^2 \sum_{l_1 l_2 l_3} l_1^4 \frac{\partial^2 \phi}{(\partial r^2)^2} + (1/2) \sum_{l_1 l_2 l_3} l_1^2 \frac{\partial \phi}{\partial r^2}, \tag{12}$$

$$B_{22} = a_2^2 \sum_{l_1 l_2 l_3} l_2^4 \frac{\partial^2 \phi}{(\partial r^2)^2} + (1/2) \sum_{l_1 l_2 l_3} l_2^2 \frac{\partial \phi}{\partial r^2}, \tag{13}$$

$$B_{12} = a_1 a_2 \sum_{l_1 l_2 l_3} l_1^2 l_2^2 \frac{\partial^2 \phi}{(\partial r^2)^2}, \tag{14}$$

$$B_{23} = a_2 a_3 \sum_{l_1 l_2 l} l_2^2 l_3^2 \frac{\partial^2 \phi}{(\partial r^2)^2}, \tag{15}$$

where a_1 and a_2 stand for semi-lattice constants and for a tetragonal crystal lattice

$$r = \left[l_1^2 a_1^2 + \left(l_2^2 + l_3^2\right) a_2^2\right]^{1/2}. \tag{16}$$

3. Computations

The behaviour of *bcc* In-Tl alloy is studied for (100) uniaxial tensile and compressive stresseses. In order to compute the theoretical strength and stability, the condition of lattice equilibrium $\partial E/\partial a_1 = \partial E/\partial a_2 = \partial E/\partial a_3 = 0$ is satisfied at experimentally known equilibrium values of semi lattice constants $a_1 = a_2 = a_3 = a^0$. Then the semi lattice constant a_1 is given small increments and decrements such that symmetrical changes in a_2 and a_3 satisfy $\partial E/\partial a_2 = \partial E/\partial a_3 = 0$ at each stage of deformation in a_1. The process of iteration has been applied to carry out these computations and continued until one of the stability conditions [eq. (3) to eq. (5)] is violated. The value of $F_1^f/(a_2^f)^2$ at which the *instability* occurs is the *theoretical strength (stress)* of the crystal and $(a_1^f - a_1^0)/a_1^0$ is the *theoretical maximal strain,* where *f* refers to the final stage at which instability occurs.

For a tensile force, the edge a_1 will elongate and the edges a_2 and a_3 will contract such that $a_2 = a_3$ and $a_4 = a_5 = a_6 = \pi/2$. Then, the deformed lattice of the alloy will possess *"tetragonal symmetry"* on violating the condition defined by eq. (5) and *bcc* In-Tl alloy is then said to have transformed into *bct*phase, as a result of the *nucleation* of its lattice. Similarly, for a compressive force, the reverse will be the effect of *nucleation* when eq. (4) is violated. At each stage of deformation, the numerical values of the modulii B_{ij}, applied stress and internal energy are calculated.

4. Results and discussion

A close survey of the literature reveals that :

(i) a wide variety of materials (both metals and alloys) have not been studied experimentally to determine their mechanical strength and stability under different modes of failure.

(ii) a sufficient number of theoretical investigations of strength and stability have not been carried out in different modes of applied stress.

(iii) a variety of metallic whiskers have exhibited maximum stresses in the range of about $0.17\ E + 10\ N/m^2$ (for Ag) to about $1.31\ E + 10\ N/m^2$ (for Fe) with a corresponding strains estimated to be about 3% to 5% [12,13].

Therefore, a detailed quantitative comparison between the theoretical and experimental behaviour in a particular failure mode is difficult to made. Even though, the effect of nucleation is manifested in the form of phase transition from *bcc* to *bct* structure under Born stability criteria.

The instability in compression and in tension for the *bcc* lattice of In-Tl alloy results from the violation of the conditions defined by eq. (4) and eq. (5) respectively.

The *bct* lattice of In-Tl alloy fails in compression by violating the condition defined by eq. (5) as a result of its inability to support an additional compressive load, while in tension by violating the condition $B_{23} > 0$ wherein the angle a_4 (the angle between a_2 and a_3) deviates from 90°.

We now discuss below our findings for *bcc* and *bct* phases of In-Tl alloy in the framework of extended generalised exponential potential, concerning the modulii B_{ij}, applied stress and internal energy.

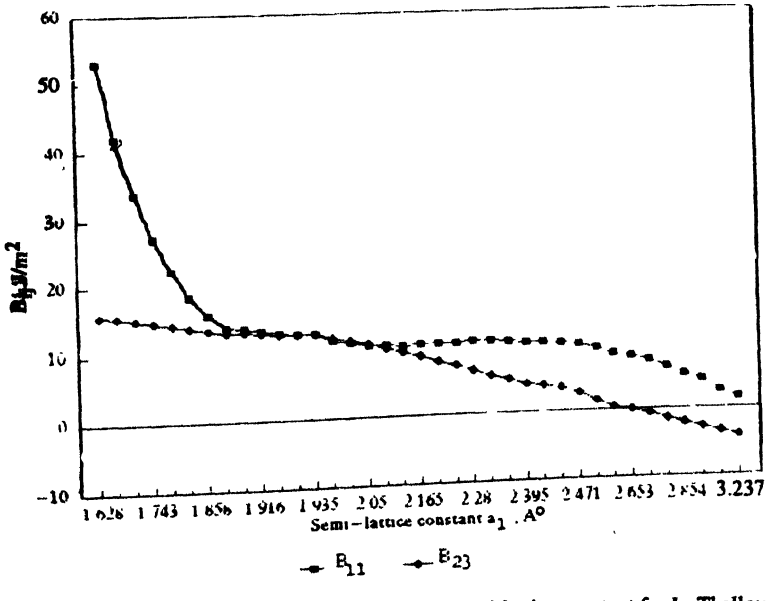

Figure 1. Variation of B_{11} and B_{23} as a function of semi-lattice constant for In-Tl alloy.

Figures 1 and 2 show the variation of B_{ij} as a function of semi lattice constant a_1 for In-Tl alloy. Figure 3 shows the variation of $AA = (B_{22} - B_{23})$ and $BB = [B_{11}(B_{22} + B_{23}) - 2B_{12}^2]$ as a function of semi lattice constant a_1 for the alloy of present concern.

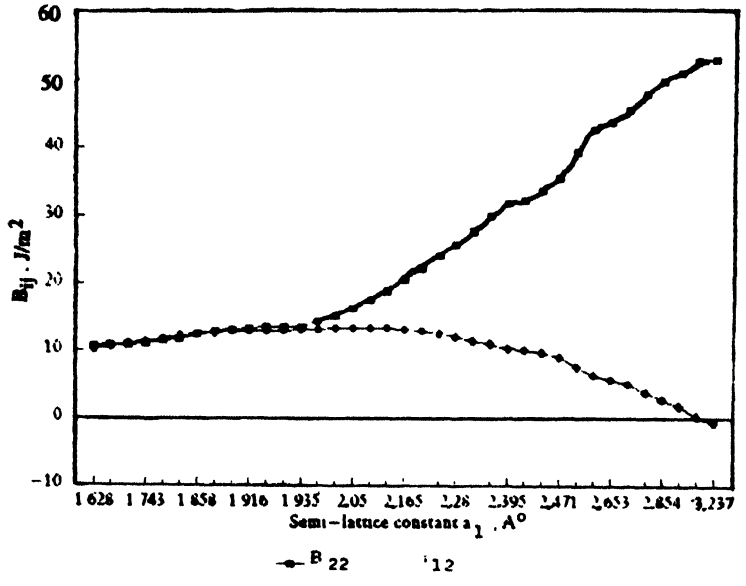

Figure 2. Variation of B_{22} and B_{12} as a function of semi-lattice constant for In-Tl alloy.

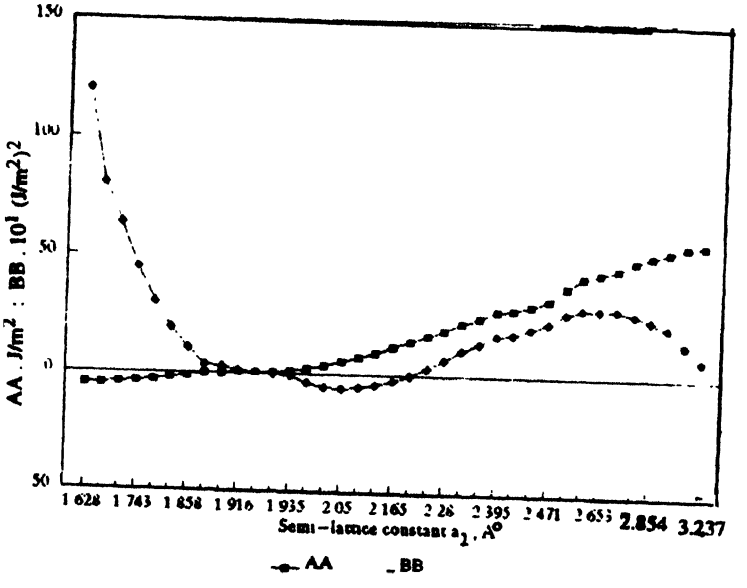

Figure 3. Variation of *AA* and *BB* as a function of semi-lattice constant for In-Tl alloy.

Figure 4 shows the variation of applied stress and internal energy of In-Tl alloy as a function of semi lattice constant a_1. It follows from Figures 3 and 4 that *bcc* lattice of In-Tl

alloy becomes unstable at a theroretical tensile stress of 0.14262 $E + 08$ N/m^2 and a corresponding strain of 0.75% when $BB < 0$ and in compression, the *bcc* lattice of In-Tl alloy becomes unstable at an applied stress of -0.15582 $E + 08$ N/m^2 with a strain of 0.6% when $AA < 0$ for $n = 3$, $m = 1.5$ and $a/a_0 = 2.2471$. Thus the range of stability of In-Tl alloy is from $a_1 = 1.904106$ Å, $a_2 = 1.921273$ Å to $a_1 = 1.929967$ Å, $a_2 = 1.908503$ Å.

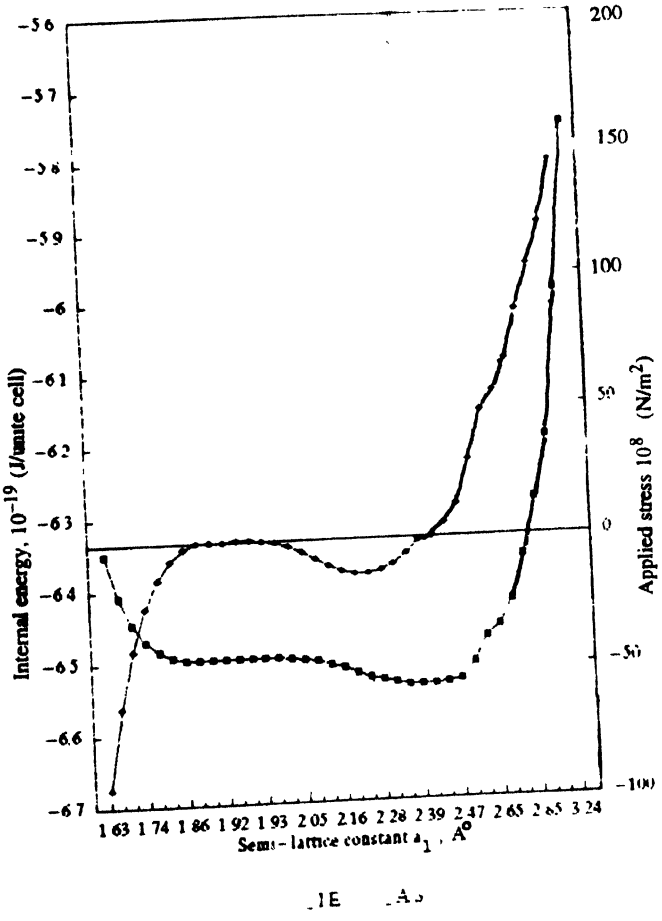

Figure 4. Variation of internal energy and applied stress as a function of semi-lattice constant for In-Tl alloy.

It follows from Figure 4 that the theoretical strength of *bct* phase of In-Tl alloy is 5.49975 $E + 09$ N/m^2 in tension when $B_{23} < 0$ and -1.37057 $E + 09$ N/m^2 in compression when eq. (5) is violated; the corresponding strains being 10.376% in tension and –6.758% in compression. The *bct* phase of In-Tl alloy is stable within the range of semi lattice constants $a_1 = 2.241252$ Å, $a_2 = 1.761274$ Å to $a_1 = 2.653106$ Å, $a_2 = 1.650335$ Å.

5. Conclusions

The following main conclusions emerges on the basis of our investigations carried out for *bcc* In-Tl alloy :

(i) The variation of internal energy defined by eq. (7) with semi lattice constant a_1 for the *bcc* In-Tl alloy under study shows *two distinct minima*, one for *bcc* phase (where stress σ_1 becomes negative) and the other for *bct* phase (where stress $\sigma_1 = 0$). It is to be noted that the internal energy minimum (IEM) of the *bct* phase is considerably lower than that of the *bcc* phase. The unstressed ($\sigma_1 = 0$) *bct* phase possesses the semi lattice constant $a_1 = b_1^0$ and $a_2 = b_2^0$ corresponding to the minimum of internal energy. The values of semi lattice constants a_1, a_2 and the corresponding values of the energy minima for the *bcc* and *bct* phases of the alloy studied are given in Table 3.

Table 1. Input data for *bcc* In-Tl alloy after [15].

Composition (at. % Tl)	Temperature (°K)	Semi-lattice constant $\times 10^{-10}$ m	Bulk modulus $\times 10^{11}$ N/m^2
76.5	300	1 9156	0.338

Table 2. Computed potential parameters for *bcc* In-Tl alloy

n	m	αa_0	$\alpha \times 10^{10}$ m^{-1}	$\beta \times 10^{09}$	$D \times 10^{-30}$ J	$r_0 \times 10^{-09}$ m
3	1.5	2.2471	1.173053	1.211624	8.311329	1.782974

Table 3. Internal energy minima (IEM) and stress of In-Tl alloy.

(a) *bcc* phase			
a_1 Å	a_2 Å	Minima position 10^{-19} J/unit cell	Stress 10^{08} N/m^2
1.953912	1.896633	–6.49731	–0.09468
(b) *bct* phase			
$a_1 = b_1^0$ Å	$a_2 = b_2^0$ Å	Minima position 10^{-19} J/unit cell	Stress 10^9 N/m^2
2..403695	1.704310	–6.54017	0.0

(ii) It follows from the analysis of our results mentioned in section 4 for the *bcc* alloy studied that the range of stability of the *bct* phase is considerably greater than that of the *bcc* phase.

(iii) The second-order elastic constants (Table 4) C_{11} and C_{12} are calculated as per Milstein [10] at the stress-free equilibrium value of semi lattice constant and at failure in tension and compression values of semi lattice constant. It is observed that the values of elastic constants (C_{11} and C_{12}) decreases in tension but in compression, the value of C_{11} increases while that of C_{12} first increases and then decreases due to the effect of ***nucleation*** for *bcc* phase. But for *bct* phase, the values of elastic constants decreases in tension while increases in compression.

Table 4. Computed values of C_{11} and C_{12} for In-Tl alloy in 10^{10} N/m^2

	(a) *bcc* phase		
	C_{11}	C_{12}	Remark
	3.43283	3.34623	At equilibrium
	3.28148	3.34229	At failure in tension
	3.56988	3.34779	At failure in compression
Expt.	3.611	3.267	[15]
	(b) *bct* phase		
	2.18287	2.09222	At equilibrium
	1.41262	1.05903	At failure in tension
	2.44737	2.75515	At failure in compression

(iv) The nature of the Figures 1 to 4 representing the variation of the moduli B_{ij}, the conditions defined by eqs. (4) and (5) and internal energy and applied stress defined by eqs. (7) and (8) with respect to semi-lattice constant a_1 show the non-linear behaviour of these properties under nucleation. The non-linear behaviour of said properties may be attributed in general to the anharmonic nature of the interactions involved, which have been embodied in the present potential implicitly [14].

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