

EFFECT OF NUCLEATION ON THE STABILITY OF BCC METALS

A. VERMA, M.L. VERMA

Department of Physics, G.G.D.S.D. College, Palwal-121102, India

AND R.P.S. RATHORE

Department of Physics, R.B.S. College, Agra-282002, India

(Received October 18, 1996)

Numerical calculations are made of theoretical strength and range of stability of a perfect uniaxially stressed crystal lattice of bcc vanadium, niobium and tantalum in the framework of extended generalised exponential potential by applying Born stability criteria. Two ranges of stability, a bcc phase and a body centered tetragonal phase are found to exist. The computed values of theoretical strength and strain of bcc V, Nb and Ta agree reasonably well with the experimental limits.

PACS numbers: 62.20.Dc

1. Introduction

The theoretical or ideal strength of a perfect crystal is defined as the strength at which a perfect lattice becomes mechanically unstable [1]. Since a perfect crystal is homogeneous throughout, it cannot become mechanically unstable till the system lowers its total energy by spontaneously undergoing uniform deformations. These deformations called *twinning or nucleation* [2] leading to structural transition from tetragonal to orthorhombic phase have direct bearing on the process of hot superconductors. The present study, however, deals with the problem of theoretical strength and stability of bcc V, Nb and Ta under *nucleation* from cubic to tetragonal phase. In fact, the theoretical strength represents an upper bound or limit to the actual strength of the crystalline solids, therefore its calculation is a problem of central importance and assumes interesting dimensions because it is thought that the strength of some metallic whiskers or fine filaments approach the theoretical limit. Before the development of the high-strength crystalline whiskers, this problem was of prime importance since the calculated values of tensile strength [3-6] were typically greater than the experimental ones by a factor of 100 or more.

Currently, this problem is still of theoretical as well as practical interest because there now exists means for obtaining high-strength crystalline whiskers which are evidently relatively free from microscopic defects (i.e. devoid of impurities and lattice imperfections). In addition, the problem of calculating the theoretical strength of perfect crystals is relevant to our understanding of many phenomena occurring in solid state physics such as:

- (i) the nature of a material whether brittle or ductile [4, 7];
- (ii) the definition of dislocation core radii [8, 9];
- (iii) the loss of coherency occurring at particle matrix interfaces [10, 11]

are the problems which involve the ideal strength of solids. Many workers [12-16] have studied this problem of theoretical strength both for undeformed and deformed crystal lattices with various modes of deformations and with various forms of interactions between the atoms. Recently, Singh [17] has computed theoretical strength of noble metals in [100] direction by using a pseudopotential approach and has made a rigorous estimation of binding energy. Probably, the present knowledge of interatomic interactions in solids is still insufficient and an accurate quantitative calculation of the theoretical strength for most of the solids is hardly tractable.

The purpose of present communication is to apply Born stability criteria [1] using the extended generalised exponential potential (EGEP) to the problem involving any kind of lattice deformation, that is, either homogeneous expansion or contraction and interpret the results of detailed numerical computations carried out for bcc vanadium, niobium and tantalum. The present potential [18] has earlier explained not only the elastic and dynamical behaviour of bcc V and Nb but also of fcc Al recently. The computed values of theoretical strength and strain for bcc V, Nb and Ta agree reasonably well with the experimental limits.

2. Theory

2.1. Extended generalised exponential potential

The attractive as well as the repulsive components of the generalised exponential potential [19] have been extended for representing their true and realistic nature. Extended generalised form of exponential potential coupling the i -th and j -th atoms separated by a distance r_{ij} assumes the form

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

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 take care of electronic exchange and correlation effects and the three-body forces such as volume forces in an alternative and simpler form respectively, D is the dissociation energy, α — the hardness parameter, r_0 — the equilibrium separation parameter and r_j is the distance of the j -th atom from the origin given by

$$r_j = (l_1^2 + l_2^2 + l_3^2)^{1/2} a_0 = L_j a_0, \quad (3)$$

where l_1 , l_2 , and l_3 (either all even or all odd for a bcc lattice) are the integers of the position coordinates and the value of j varies from 1 to 306 atoms.

Equation (2) can be put in the form to represent the cohesive energy at equilibrium semi-lattice constant (a_0) as below

$$\Phi(a_0) = [D/2(m-1)] \times \left[\beta^m (\alpha a_0)^{-n} \sum_{l_1 l_2 l_3} L_j^{-n} e^{-m\alpha a_0 L_j} - m\beta (\alpha a_0)^n \sum_{l_1 l_2 l_3} L_j^n e^{-\alpha a_0 L_j} \right], \quad (4)$$

where

$$\beta = \exp(\alpha r_0). \quad (5)$$

The three defining parameters (α , r_0 , and D) of the potential require for their evaluation the precisely determined input data of equilibrium semi-lattice constant (a_0) and bulk modulus (B) of the metals only (Table I). For evaluating the three parameters α , r_0 and D of the potential function, the condition [19]

$$\sum_{l_1 l_2 l_3} [l_1^2 d\Phi(r)/dr^2] = 0 \quad (6)$$

for the equilibrium of the crystal in the absence of external forces was employed and executed (Table II).

TABLE I

Input data for bcc metals.

Metal	Semi-lattice constant [$\times 10^{-10}$ m]	Bulk modulus [$\times 10^{11}$ N/m ²]
V	1.515	1.619
Nb	1.650	1.702
Ta	1.650	2.000

TABLE II

Computed potential parameters for bcc metals.

Metal	n	m	αa_0	α [$\times 10^{10}$ m ⁻¹]	β	D [$\times 10^{-26}$ J]	r_0 [$\times 10^{-9}$ m]
V	2	1.5	2.0989	1.385413	2186878	5.943871	1.053692
Nb	2	1.5	2.0194	1.223879	1594490	10.324240	1.166950
Ta	2	1.5	2.1719	1.316303	2923407	7.549511	1.131066

2.2 Theoretical considerations

The present calculations are based on the theory and procedure proposed by Milstein [13] in considerable detail for applying the Born stability criteria to the determination of the mechanical stability of cubic crystals in the presence of

applied forces and deformations. Therefore, only few essential aspects are mentioned here. For [100] uniaxial stress in cubic crystals with central interactions, the necessary and sufficient conditions for a lattice to be in stable equilibrium are

$$B_{11} > 0, \quad B_{22} > 0, \quad B_{12} > 0, \quad B_{23} > 0, \quad (7)$$

$$AA = B_{22} - B_{23} > 0, \quad (8)$$

$$BB = B_{11}(B_{22} + B_{23}) - 2(B_{12})^2 > 0, \quad (9)$$

where

$$B_{ij} = \frac{\partial^2 E}{\partial a_i \partial a_j} \quad (10)$$

and E is the energy per unit cell given by

$$E = (1/2)n' \sum_{l_1 l_2 l_3} \phi(r). \quad (11)$$

i and j have their values ranging from 1 to 6 and n' is the number of atoms per unit cell. a_1 , a_2 and a_3 are the edges of the unit cell and a_4 , a_5 and a_6 are the angles between half the edges 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

$$\sigma = \frac{1}{a_2 a_3} \left[\frac{\partial E}{\partial a_1} \right]. \quad (12)$$

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

$$F_1 = \left[\frac{\partial E}{\partial a_1} \right] \quad (13)$$

and the force F_2 acting along a_2 is

$$F_2 = \left[\frac{\partial E}{\partial a_2} \right] = 0, \quad (14)$$

where for a tetragonal crystal lattice

$$a_2 = a_3 \quad \text{and} \quad a_4 = a_5 = a_6 = \pi/2. \quad (15)$$

The moduli B_{ij} embodied in Eqs. (7) to (9) are given by (with $n' = 2$ for bcc lattice)

$$B_{11} = a_1^2 \sum_{l_1 l_2 l_3} l_1^4 \frac{\partial^2 \phi}{(\partial r^2)^2} + (1/2) \sum_{l_1 l_2 l_3} l_1^2 \frac{\partial \phi}{\partial r^2}, \quad (16)$$

$$B_{22} = a_2^2 \sum_{l_1 l_2 l_3} l_2^4 \frac{\partial^2 \phi}{(\partial r^2)^2} + (1/2) \sum_{l_1 l_2 l_3} l_2^2 \frac{\partial \phi}{\partial r^2}, \quad (17)$$

$$B_{12} = a_1 a_2 \sum_{l_1 l_2 l_3} l_1^2 l_2^2 \frac{\partial^2 \phi}{(\partial r^2)^2}, \quad (18)$$

$$B_{23} = a_2 a_3 \sum_{l_1 l_2 l_3} l_2^2 l_3^2 \frac{\partial^2 \phi}{(\partial r^2)^2}, \quad (19)$$

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

$$r = [l_1^2 a_1^2 + (l_2^2 + l_3^2) a_2^2]^{1/2}. \quad (20)$$

3. Computations and results

The behaviour of perfect bcc crystals of V, Nb and Ta are studied for (100) uniaxial tensile and compressive stresses. 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 $a_1 = a_2 = a_3 = a^0$. Under the action of force F_1 (Eq. (13)), the semi-lattice constant a_1 is given small increments and decrements to make *nucleation* effective 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 was applied to carry out these computations and continued until one of the stability conditions (Eq. (7) to Eq. (9)) 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 crystal will possess "*tetragonal symmetry*" and bcc crystal lattice transforms into body centered tetragonal (bct) phase, as a result of *nucleation* of the crystal lattice. Similarly, for a compressive force, the reverse will be the effect of *nucleation*. At each stage of deformation, the numerical values of the moduli B_{ij} , applied stress and internal energy are calculated.

4. Conclusions

A close survey of the literature reveals that even today, there exist not enough experimental data on a wide variety of materials, involving different modes of failure, nor there has been a sufficient number of theoretical calculations of stability, in different modes of applied stress, to make detailed quantitative comparison between the theoretical and experimental behaviour in particular failure modes. Nevertheless, it is still satisfying to note that a variety of metallic whiskers have exhibited maximum stresses in the range of about 0.17×10^{10} N/m² (for Ag) to about 1.31×10^{10} N/m² (for Fe) with a corresponding strains estimated to be about 3% to 5% [20-22].

The effect of *nucleation* i.e. instability in tension for the bcc lattice results from the violation of the condition defined by Eq. (9). Evidently this relation (Eq. (9)) becomes violated when a further increase in semi-lattice constant a_1 leads to a decrease in the equilibrium stress i.e. when the lattice cannot accommodate a further increase in applied stress.

The effect of *nucleation* i.e. instability in compression for the bcc lattice results from the violation of the condition defined by Eq. (8). The violation of this

condition corresponds to the mode of failure by which the crystal can lower its total energy by undergoing spontaneously the following lattice deformation.

The variation of internal energy defined by Eq. (11) with semi-lattice constant a_1 for the bcc metals 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 metals studied are given in Table III.

TABLE III

Internal energy minima (IEM) and stress.

(a) bcc phase				
Metal	a_1 [Å]	a_2 [Å]	Minima position [10^{-19} J/unit cell]	Stress [10^9 N/m ²]
V	1.59075	1.478295	-16.991	-0.0468
Nb	1.76550	1.594449	-24.224	-0.5077
Ta	1.73250	1.609795	-25.920	-0.3241
(b) bct phase				
Metal	$a_1 = b_1^0$ [Å]	$a_2 = b_2^0$ [Å]	Minima position [10^{-19} J/unit cell]	Stress [10^9 N/m ²]
V	1.931625	1.338190	-17.079	0.0
Nb	2.095500	1.459299	-24.319	0.0
Ta	2.163750	1.456480	-26.069	0.0

The bct lattice fails in tension due to *increased nucleation* by violating the condition $B_{23} > 0$. When this condition is violated, the lattice can lower its energy by undergoing a spontaneous deformation wherein the angle a_4 (the angle between a_2 and a_3) deviates from 90° .

The bct lattice fails in compression due to *increased nucleation* by violating the condition defined by Eq. (9). The violation of this condition results when the lattice cannot support an additional compressive load i.e. when a decrease in semi-lattice constant a_1 results in an increase rather than a decrease in stress σ_1 .

It is to be noted that the range of stability of the bct phase is considerably greater than that of the bcc phase.

We now discuss below our findings for bcc metallic crystals in the framework of extended generalised exponential potential, concerning the moduli B_{ij} , applied stress and internal energy.

4.1. Vanadium

Figures 1 and 2 show the variation of B_{ij} as a function of semi-lattice constant a_1 for V. 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 V. Figure 4 shows the variation of applied stress and internal energy of V as a function of semi-lattice constant a_1 . It follows from Fig. 3 and Fig. 4 that bcc lattice of V becomes unstable at a theoretical tensile stress of 0.4698×10^9 N/m² and a corresponding strain of 1.75% when $BB < 0$ and in compression, the bcc lattice of V becomes unstable at an applied stress of -0.7466×10^9 N/m² with a strain of 1.65% when $AA < 0$ for $n = 2$, $m = 1.5$ and $\alpha a_0 = 2.0989$. Thus the range of stability of V is from $a_1 = 1.541513$ Å, $a_2 = 1.502205$ Å to $a_1 = 1.490003$ Å, $a_2 = 1.527006$ Å.

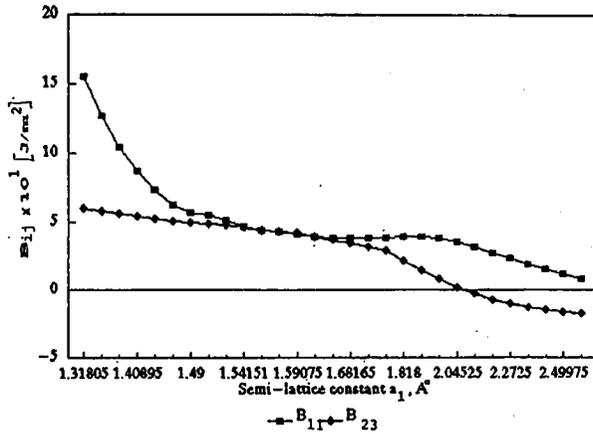


Fig. 1. Variation of B_{11} and B_{23} as a function of semi-lattice constant for V.

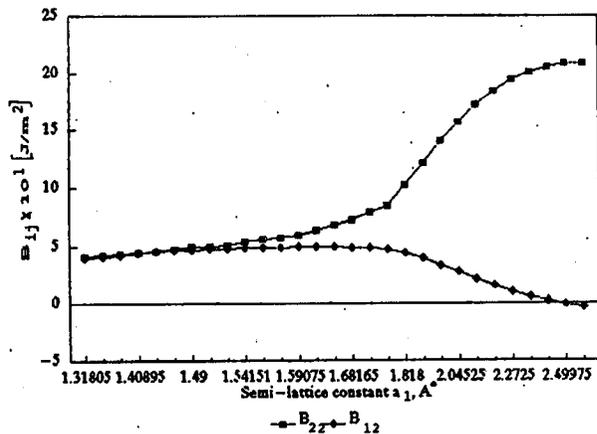


Fig. 2. Variation of B_{22} and B_{12} as a function of semi-lattice constant for V.

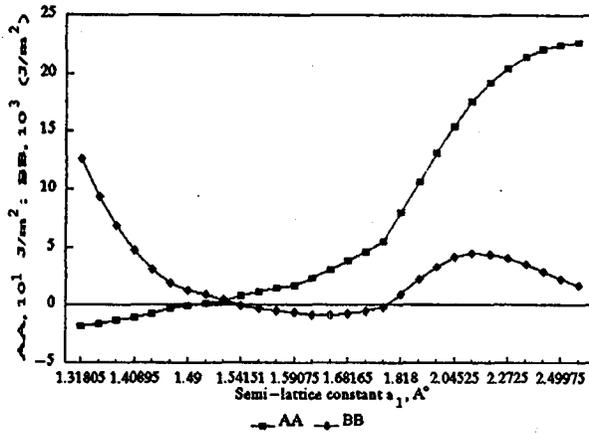


Fig. 3. Variation of AA and BB as a function of semi-lattice constant for V.

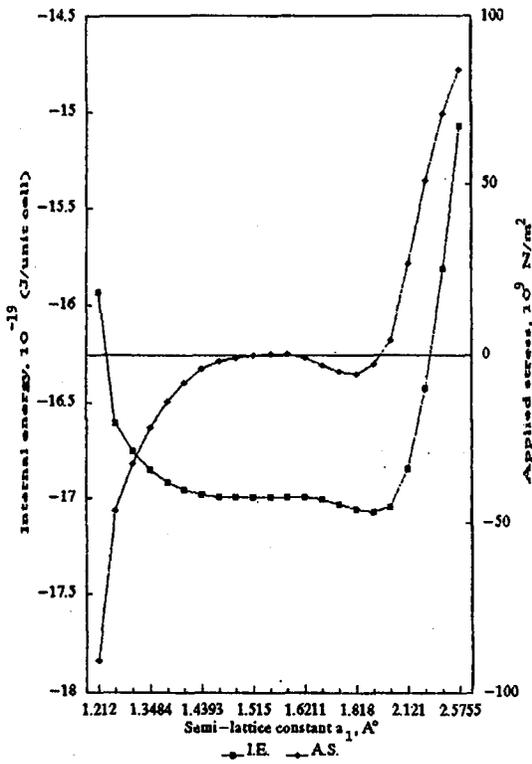


Fig. 4. Variation of internal energy and applied stress as a function of semi-lattice constant for V.

It follows from Fig. 4 that the theoretical strength of bct phase of V is 2.065×10^{10} N/m² in tension when $B_{23} < 0$ and -0.56×10^{10} N/m² in compression when Eq. (9) is violated; the corresponding strains being 7.84% in tension and -5.88% in compression. The bct phase of V is stable within the range of semi-lattice constants $a_1 = 1.818 \text{ \AA}$, $a_2 = 1.37624 \text{ \AA}$ to $a_1 = 2.083125 \text{ \AA}$, $a_2 = 1.30338 \text{ \AA}$.

4.2. Niobium

Figures 5 and 6 show the variation of B_{ij} as a function of semi-lattice constant a_1 for Nb. Figure 7 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 Nb. Figure 8 shows the variation of applied stress and internal energy of Nb as a function of semi-lattice constant a_1 . Figures 7 and 8 show that bcc lattice of

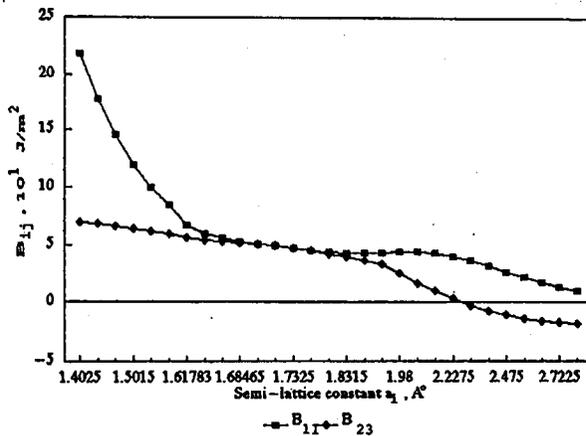


Fig. 5. Variation of B_{11} and B_{23} a function of semi-lattice constant for Nb.

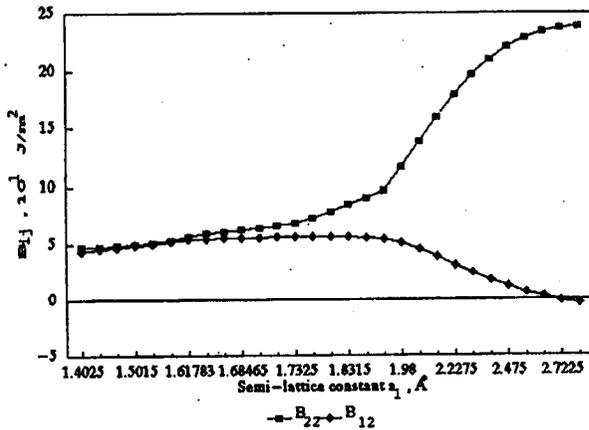


Fig. 6. Variation of B_{22} and B_{12} as a function of semi-lattice constant for Nb.

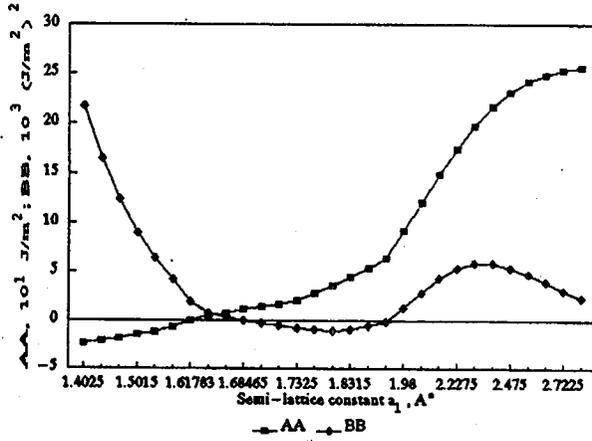


Fig. 7. Variation of AA and BB as a function of semi-lattice constant for Nb.

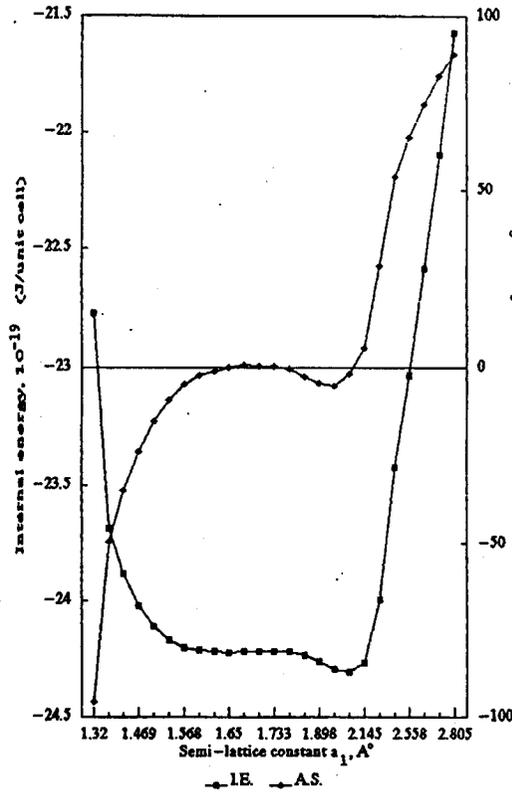


Fig. 8. Variation of internal energy and applied stress as a function of semi-lattice constant for Nb.

Nb becomes unstable at a theoretical tensile stress of $0.6875 \times 10^9 \text{ N/m}^2$ and a corresponding strain of 2.1% when $BB < 0$ and in compression, the bcc lattice of Nb becomes unstable at an applied stress of $-1.1017 \times 10^9 \text{ N/m}^2$ with a strain of 1.95% when $AA < 0$ for $n = 2$, $m = 1.5$ and $\alpha a_0 = 2.0194$. Thus the range of stability of Nb is from $a_1 = 1.68465 \text{ \AA}$, $a_2 = 1.633385 \text{ \AA}$ to $a_1 = 1.617825 \text{ \AA}$, $a_2 = 1.665341 \text{ \AA}$.

Figure 8 shows that the theoretical strength of bct phase of Nb is $2.2 \times 10^{10} \text{ N/m}^2$ in tension when $B_{23} < 0$ and $-0.499 \times 10^{10} \text{ N/m}^2$ in compression when Eq. (9) is violated; the corresponding strains 8.27% in tension and -5.51% in compression. The bct phase of Nb is stable within the range of semi-lattice constants $a_1 = 1.98 \text{ \AA}$, $a_2 = 1.499948 \text{ \AA}$ to $a_1 = 2.26875 \text{ \AA}$, $a_2 = 1.420672 \text{ \AA}$.

4.3. Tantalum

Figures 9 and 10 exhibit the variation of B_{ij} as a function of semi-lattice constant a_1 for bcc Ta. Figure 11 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 bcc Ta. Figure 12 shows the variation of applied stress and internal energy of bcc Ta as a function of semi-lattice constant a_1 . It follows from Fig. 11 and Fig. 12 that bcc lattice of Ta becomes unstable at a theoretical tensile stress of $0.4339 \times 10^9 \text{ N/m}^2$ and a corresponding strain of 1.47% when $BB < 0$ and in compression, the bcc lattice of Ta becomes unstable at an applied stress of $-0.6599 \times 10^9 \text{ N/m}^2$ with a strain of 1.38% when $AA < 0$ for $n = 2$, $m = 1.5$ and $\alpha a_0 = 2.1719$. Thus the range of stability of bcc Ta is from $a_1 = 1.674255 \text{ \AA}$, $a_2 = 1.638234 \text{ \AA}$ to $a_1 = 1.62723 \text{ \AA}$, $a_2 = 1.661007 \text{ \AA}$.

It follows from Fig. 12 that the theoretical strength of bct phase of Ta is $2.35 \times 10^{10} \text{ N/m}^2$ in tension when $B_{23} < 0$ and $-0.785 \times 10^{10} \text{ N/m}^2$ in compression when Eq. (9) is violated; the corresponding strains 7.45% in tension and -5.88%

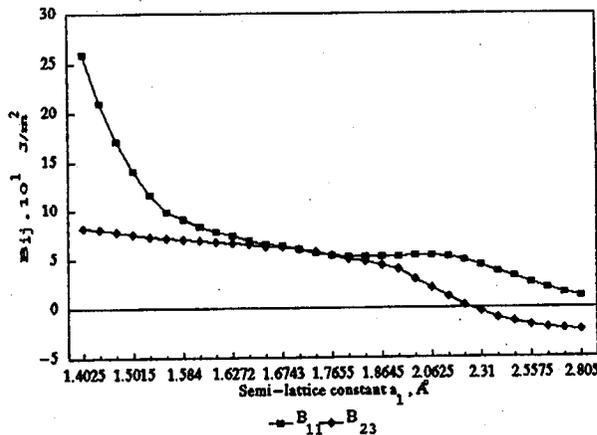


Fig. 9. Variation of B_{11} and B_{23} as a function of semi-lattice constant for Ta.

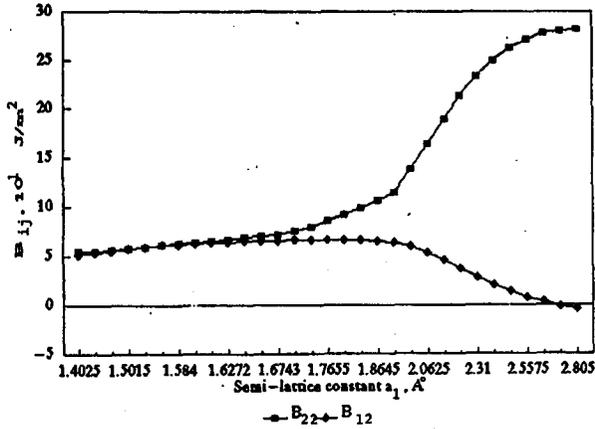


Fig. 10. Variation of B_{22} and B_{12} as a function of semi-lattice constant for Ta.

TABLE IV
Computed values of C_{11} and C_{12} for bcc phase in 10^{11} N/m².

Metal	C_{11}	C_{12}	Remark
V	1.6974	1.5769	At equilibrium
	1.5221	1.5713	At failure in tension
	1.9157	1.5776	At failure in compression
Expt.	2.280	1.187	[23]
	1.96	1.33	[24]
Nb	1.7994	1.6508	At equilibrium
	1.5797	1.6419	At failure in tension
	2.0815	1.6513	At failure in compression
Expt.	2.46	1.34	[24]
Ta	2.0820	1.9553	At equilibrium
	1.8994	1.9503	At failure in tension
	2.2997	1.9561	At failure in compression
Expt.	2.609	1.574	[23]

in compression. The bcc phase of Ta is stable within the range of semi-lattice constants $a_1 = 1.98 \text{ \AA}$, $a_2 = 1.498008 \text{ \AA}$ to $a_1 = 2.2605 \text{ \AA}$, $a_2 = 1.419068 \text{ \AA}$.

Finally, the second-order elastic constants (Table IV) C_{11} and C_{12} are calculated as per Milstein [13] at the stress-free equilibrium values of semi-lattice constant and at failure in tension and compression values of semi-lattice constant. It is observed that in general computed values of elastic constants (C_{11} and C_{12}) decreases in tension and increases in compression, due to the effect of *nucleation*.

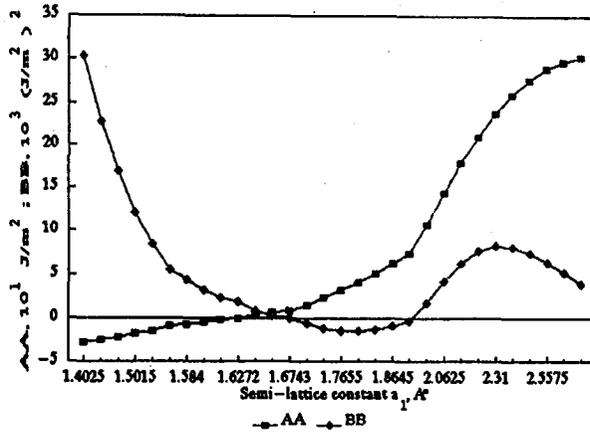


Fig. 11. Variation of AA and BB as a function of semi-lattice constant for Ta.

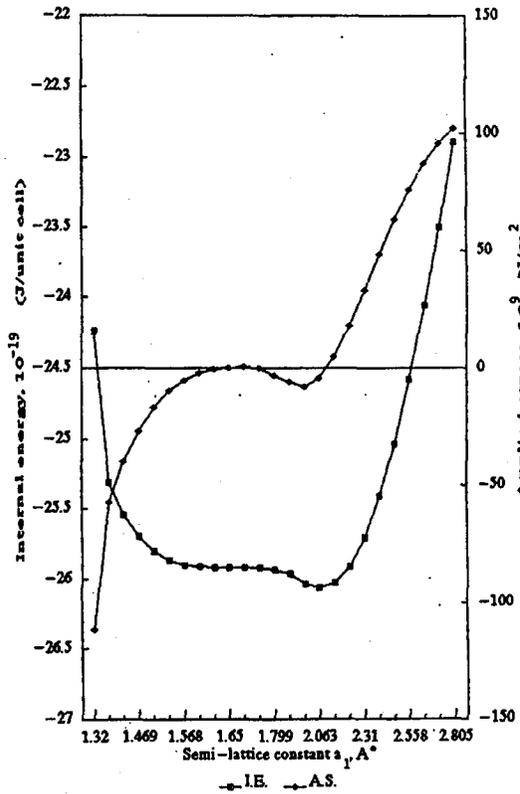


Fig. 12. Variation of internal energy and applied stress as a function of semi-lattice constant for Ta.

Acknowledgments

Two of us (A.V. and M.L.V.) are thankful to Mr. N.K. Khurana of Universal Computer Training Point (UCTP) for providing computation facility and to Dr. G. Singh, R.B.S. College, Agra, for many useful discussions.

References

- [1] M. Born, *Proc. Camb. Philos. Soc.* **36**, 160 (1940).
- [2] I.H. Khlyustkov, A.T. Buzdin, *Adv. Phys.* **36**, 271 (1987); J.G. Bednorz, K.A. Mueller, *Z. Phys. B* **64**, 189 (1986); Z.Z. Sheng, A.M. Herman, *Nature* **332**, 138 (1988).
- [3] M. Born, R. Furth, *Proc. Camb. Philos. Soc.* **36**, 454 (1940).
- [4] A. Kelly, *Strong Solids*, Clarendon Press, Oxford 1966.
- [5] W.R. Tyson, *Philos. Mag.* **14**, 925 (1966).
- [6] N.H. Macmillan, *J. Mater. Sci.* **7**, 239 (1972).
- [7] A. Kelly, W.R. Tyson, A.A. Cottrell, *Philos. Mag.* **15**, 567 (1967).
- [8] P.C. Ghlen, A.R. Rosenfield, G.T. Hahn, *J. Appl. Phys.* **39**, 5246 (1968).
- [9] Z.S. Basinski, M.S. Duesbery, R. Taylor, *Philos. Mag.* **21**, 1201 (1970).
- [10] M.F. Ashbay, S.H. Gelles, L.E. Tanner, *Philos. Mag.* **19**, 757 (1969).
- [11] L.M. Brown, G.R. Woolhouse, *Philos. Mag.* **21**, 329 (1970).
- [12] R.D. Misra, *Proc. Camb. Philos. Soc.* **36**, 173 (1940).
- [13] F. Milstein, *Phys. Rev. B* **2**, 512 (1971); *Phys. Rev. B* **3**, 1130 (1971).
- [14] F. Milstein, *Phys. Rev. B* **10**, 3635 (1974); *J. Appl. Phys.* **44**, 3833 (1973).
- [15] A.K. Mitra, P.K. Sengupta, *J. Phys. F* **13**, 2221 (1983).
- [16] G. Singh, R.P.S. Rathore, *Indian J. Pure Appl. Phys.* **24**, 303 (1986).
- [17] G. Singh, *Indian J. Pure Appl. Phys.* **28**, 122 (1990); *Phys. Status Solidi B* **161**, 145 (1990); *Phys. Status Solidi B* **164**, 401 (1991).
- [18] A. Verma, M.L. Verma, R.P.S. Rathore, *Acta Phys. Pol. A* **90**, 547 (1996); M.L. Verma, A. Verma, R.P.S. Rathore, *Indian J. Phys. A* **70**, 603 (1996).
- [19] F. Milstein, *J. Appl. Phys.* **44**, 3825 (1973).
- [20] S.S. Brenner, *J. Appl. Phys.* **27**, 1484 (1956).
- [21] S.S. Brenner, *Science* **128**, 569 (1958).
- [22] J.C. Crump, J.W. Mitchell, *J. Appl. Phys.* **41**, 717 (1970).
- [23] C. Kittel, *Introduction to Solid State Physics*, 3rd ed., Wiley, New York 1968, p. 122.
- [24] I.D. Bolef, *J. Appl. Phys.* **32**, 100 (1961).