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LATTICE VIBRATION ASPECT OF SOME METALLURGICAL PROPERTIES OF CUBIC CRYSTALS

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The Debye-Waller thermal parameter B is a measure of the mean-square amplitude of atomic vibrations $\langle u^2 \rangle$. For monoatomic cubic crystals in which the vibrations are isotropic, $B = 8\pi\langle u^2\rangle/3$. In this study, it is observed that various metallurgical properties, e.g., ultimate tensile strength, creep-onset temperature, recrystallisation temperature, activation energy for grain boundary self-diffusion, solubility limit, etc. of cubic elements are a unique function of their B-factors. The power regression formula $Y = Y_0(B/B_0)^M$ depicts the correlation between a metallurgical property Y and the Debye-Waller thermal parameter B. The regression coefficient Y_0 and regression power M are determined by the least-squares method, while B_0 is a constant which makes the equation dimensionally homogeneous.

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1. Introduction

The study of relationship between the microscopic properties based on single-atom behaviour of a material and the macroscopic properties involving a bulk has proved to be quite useful in understanding and interpreting the overall behaviour of materials. In particular, the correlations of the Debye-Waller thermal parameter B with several bulk properties of 20 cubic elements [1-7] are innovative in relation to the practical as well theoretical aspects of physics, providing a sound base for extensive future research. Such investigations were also carried out in the case of 58 cubic compounds [8-10].

To illustrate the significance of such studies, it will suffice to quote the example of yield stress of metals, which is a common measure of elastic strength important to the design engineers. Butt and Chaudhary [2] have explicitly demonstrated that the B-factor of cubic metals is the most dominant parameter compared with other experimental variables, e.g., orientation of single crystals, grain size of polycrystals, elemental purity, dislocation density, strain-rate and temperature of onset of deformation, heat-treatment prior to deformation, etc., customarily taken into account in the theoretical models of yielding. They found that for a given crystal structure, metals with a high B-factor have low yield stress, which means that metallic crystals composed of atoms with large mean-square amplitude of atomic vibrations $\langle u^2 \rangle = (3/8\pi^2)\, B$ are easy to deform. Like the macroscopic yield stress, the microscopic parameters of the unit activation process of yielding postulated in the kink-pair nucleation model of plastic flow in metals [11], e.g., the initial length of dislocation segment, the critical height of the kink-pair nucleated, the associated activation volume, the binding energy per interatomic spacing along the glide dislocation on the slip plane etc. were also found [12] to correlate well with the mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ through a power regression formula. Similar results were also obtained in the case of hardness [1], activation energy of high-temperature creep [6], and stacking-fault energy/width ratio [7] in cubic metals.

Main object of the present work was to extend the investigations cited above to some other metallurgical properties of technological importance. Thus ultimate tensile strength (UTS), minimum temperature for initiation of creep (T_c), recrystallisation temperature (T_r), activation energy for grain boundary self-diffusion (H_0) in common metals as well as solubility limit (SL) of some cubic elements in copper will be studied as a function of their Debye-Waller thermal parameter B. The most accurate B values recommended by Butt et al. [13] for 22 cubic elements will be used for this purpose.

2. *Metallurgical properties versus B-factor*

2.1. *Ultimate tensile strength*

The maximum value of engineering stress that a material can withstand during a tensile test leading to fracture is called its ultimate tensile strength (UTS). Reference to Fig. 1 shows the UTS values of eight cubic metals as a function of their B-factor in double logarithmic plot. The line drawn through the data points taken from Ref. [14] was obtained by the least-squares fit method, and is given by the relation

$$UTS = 6.2 \times 10^{-2} (B/B_0)^{-1.51}\,, \tag{1}$$

with a linear correlation coefficient $r = -\,0.98$. The constant $B_0 = 1$ nm^2 has been introduced to make the equation dimensionally homogeneous. This shows that UTS of cubic metals referred to correlates very well with their B-factor. The higher the value of B or $\langle u^2 \rangle$, the lower will be the maximum engineering stress that a metal is capable of withstanding.

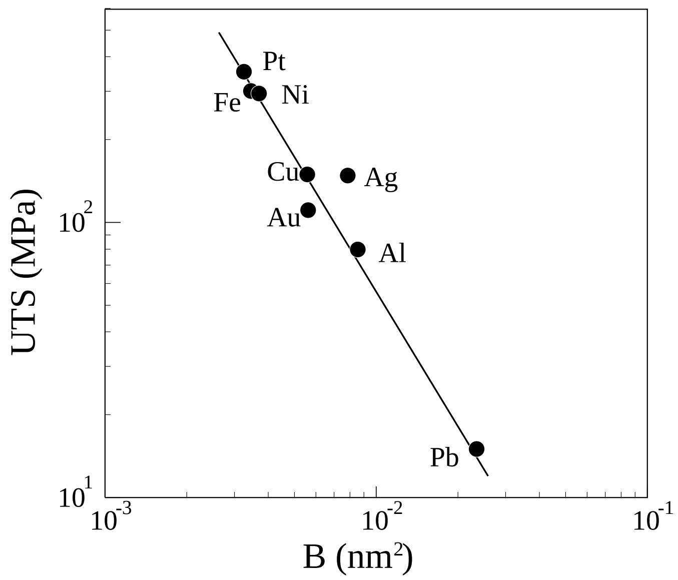

Fig. 1. Ultimate tensile strength of some cubic elements as a function of their B-factor. UTS values were taken from Ref. [14].

2.2. Creep-onset temperature

The plastic deformation within a material that occurs as function of time when that material is subjected to a constant load is called creep. The loads involved are

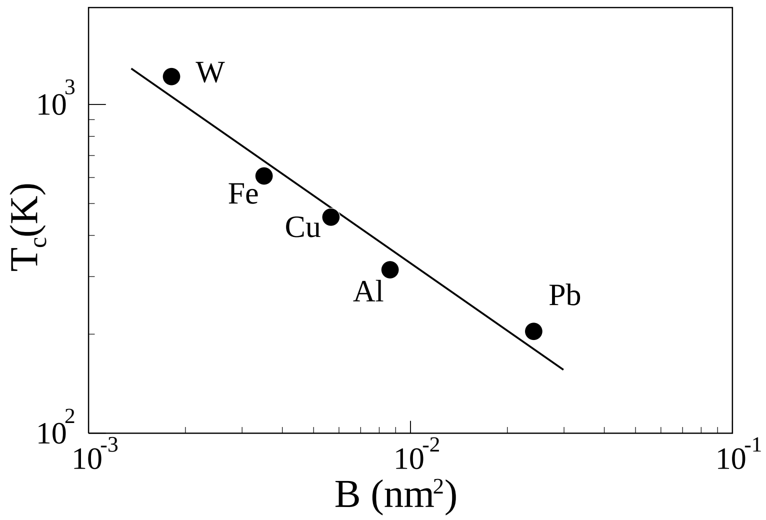

Fig. 2. Critical temperature for initiation of creep in five common cubic metals as a function of their B-factor. Data points denote T_c values taken from Ref. [15].

always much less than the elastic limit of the material at normal temperatures. It has been found that creep will not occur to any measurable extend below a certain temperature T_c, and this is different for each metal. In Fig. 2 the points represent values of the temperatures below which creep does not occur in five common metals. The straight line fitted to the data points taken from Ref. [15] was obtained by the least-squares method. It is represented by the expression

$$T_c = 14.2\,(B/B_0)^{-0.68}\,, \tag{2}$$

with a linear correlation coefficient $r = -0.98$ and constant $B_0 = 1$ nm^2. This indicates that a metal with low value of mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ requires a high temperature for the onset of creep.

2.3. Recrystallisation temperature

The nucleation and growth of stress-free grains in a deformed crystalline matrix is called recrystallisation. The lowest temperature at which recrystallisation will proceed at a reasonable rate is termed as recrystallisation temperature T_r. Figure 3 depicts, in double logarithmic plot, the recrystallisation temperatures versus B-factors of eight common metals. The data points represent the values of T_r taken from Ref. [15], while the straight line drawn through them by the least-squares fit method is represented by the equation

$$T_r = 22.6\,(B/B_0)^{-0.64}\,. \tag{3}$$

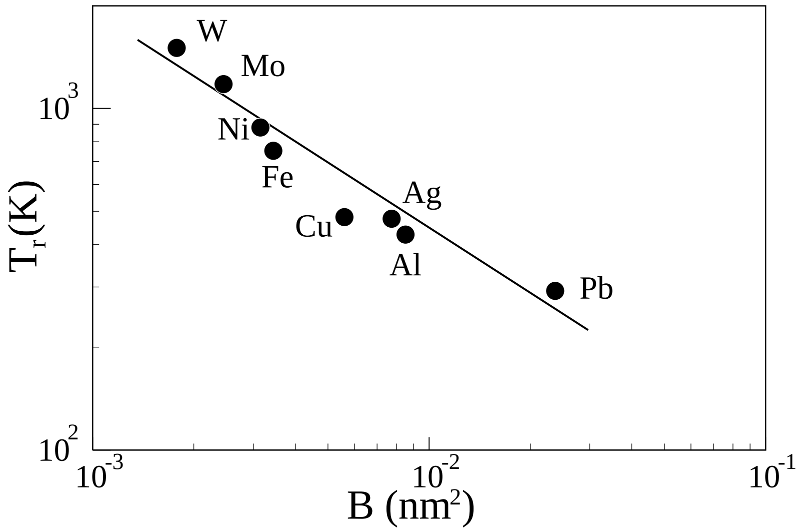

Fig. 3. Recrystallisation temperature of eight cubic elements as a function of their B-factor. Data points denote T_r values taken from Ref. [15].

2.4. Activation energy for grain growth

Grain growth in nominally pure metals has been found [16–22] to be given by the relation

$$D^2 - D_0^2 = K_0 t\,(-H_0/kT)\,, \tag{4}$$

where D and D_0 are, respectively, the instantaneous and initial mean grain-diameters, t is the time of isothermal annealing, K_0 is a constant of the order of 10^{-2} cm^2 s^{-1} and H_0 is the activation energy for grain boundary self-diffusion. The data points in Fig. 4 represent the H_0 values [19-26] for seven metals as a function of their B factors in a log-log plot.

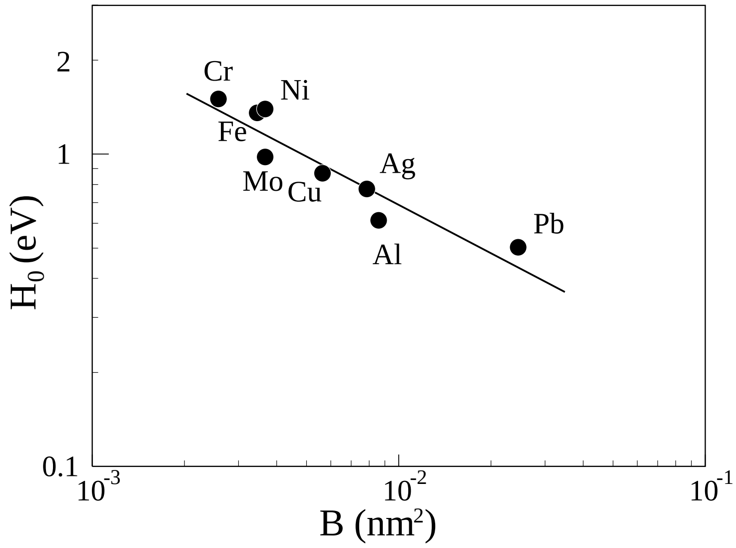

Fig. 4. Activation energy for grain boundary self-diffusion in cubic metals as a function of their B-factor. Sources of H_0 data: Cu *[19,20],* Ni *[21,25],* Al *[22],* Ag *[23],* Fe *and* Cr *[24], and* Pb *[26].*

The straight line fitted to the data points by the least-squares fit method is given by the relation

$$H_0 = 6.1 \times 10^{-2}\,(B/B_0)^{-0.53}\,, \tag{5}$$

with a correlation factor of -0.92 and constant $B_0 = 1$ nm^2. Therefore, it appears that metals composed of atoms with a high $\langle u^2 \rangle$ require less activation energy for grain-boundary self-diffusion during the process of grain growth.

2.5. Solubility limit

The maximum concentration of an element (solute), which can be mixed with a given metal (solvent) to form a primary solid-solution, where the crystal is the same as the parent metal, is called the solubility limit. According to the well known Hume-Rothery rules [27], the extent of primary solid solubility depends on (i) the difference between the atomic radii of the solute and solvent metals, (ii) their relative valences and (iii) their electrochemical difference. Figure 5 illustrates the relationship between the solubility limit SL (weight percent) of cubic elements in copper solvent. The solubility limit data taken from Ref. [28] are presented by points as a function of B-factors of the solute elements in the log-log plot. The straight line drawn through the data points with the help of the least-squares method is given by

$$SL = 9.42 \times 10^{-9} \, (B/B_0)^{-3.97} \, , \tag{6}$$

with the correlation factor $r = -0.78$ and constant $B_0 = 1$ nm^2. Equation (6) implies that an element with a rather large value of B or $\langle u^2 \rangle$ is soluble in copper to a small extent.

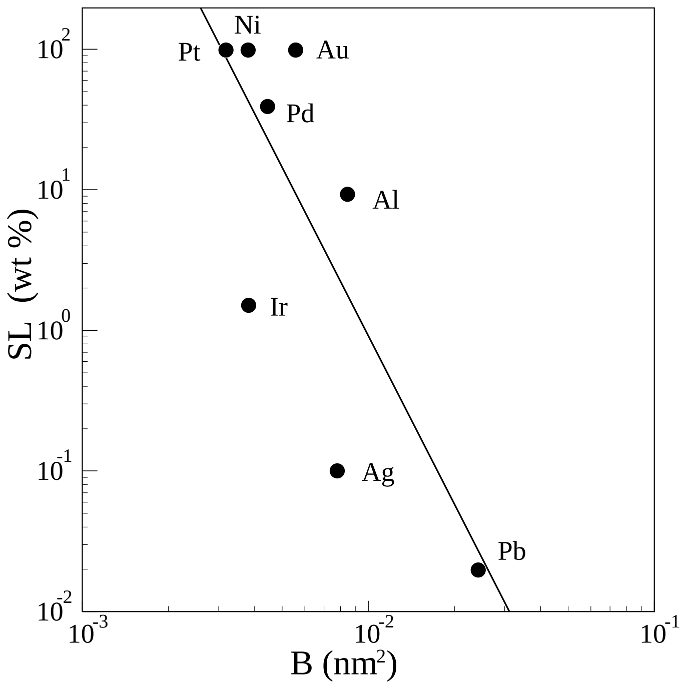

Fig. 5. Solubility limit of some cubic elements in copper as a function of their B-factor. Data points denote SL values taken from Ref. [28].

3. Conclusions

From the foregoing evidence, we conclude that the metallurgical properties, namely ultimate tensile strength, creep-onset temperature, recrystallisation temperature and activation energy for grain boundary self-diffusion in cubic metals are uniquely related to their Debye-Waller thermal parameter B through a common power-law: $Y = Y_0(B/B_0)^M$, where Y is the metallurgical property of interest, Y_0 the regression coefficient and regression power M are constants determined by the least-squares fit method, and B_0 is a constant which makes the equation dimensionally homogeneous. Knowing the value of B for a cubic element, one can predict the values of UTS, creep-onset temperature, recrystallisation temperature and activation energy for grain boundary self-diffusion for that element making use of the power-law with appropriate values of Y_0 and M. Similarly, the solubility limit of face-centred cubic elements in copper lattice also follows the same power-law.

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OVISNOST METALURŠKIH SVOJSTAVA KUBNIH KRISTALA O TITRANJU REŠETKE

Debye-Wallerov termički parametar B je mjera srednje-kvadratne amplitude atomskog titranja $\langle u^2 \rangle$. Za monoatomske kubne kristale, koji pokazuju isotropno titranje, $B = 8\pi\langle u^2\rangle/3$. U ovom se radu pokazuje kako se niz metalurških svojstava, npr., čvrstoća, temperatura pojave plastične deformacije, temperatura rekristalizacije, aktivacijska energija za difuziju kroz granice kristalića, granica topivosti i druga, elemenata kubne strukture, mogu prikazati jednim izrazom kao funkcije njihovih B-faktora. Regresijska relacija $Y = Y_0(B/B_0)^M$ daje tu korelaciju metalurškog svojstva i Debye-Wallerovog termičkog parametra B. Regresijski koeficijent Y_0 i regresijski eksponent M određuju se metodom najmanjih kvadrata, dok je B_0 konstanta kojom se postiže dimenzijska homogenost relacije.