

A Molecular-Dynamics Model for Thermal Failure of the BCC Crystal.

I. The Elastic Constants

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Abstract – The stability of the sodium crystal and its failure mechanism are investigated by the molecular dynamics method. The superheating of the bcc crystal in the model is $0.09 T_m$. On approaching the disordering temperature, T^* , first the shear modulus, $c_{11}^T - c_{12}^T$, and then c_{44}^T go to zero, whereas c_{11}^T retains a nonzero value even at T^* . The bcc crystal begins to fail with the irreversible slip of the particles in the most populated plane (110). In the metastable region, the temperature dependence of the pressure derivatives of the second-order elastic constants, as determined from the calculated second and third-order elastic constants, has a sharp peak whose position corresponds to the disordering temperature.

INTRODUCTION

When placed in isothermal conditions, free-surface crystals will melt at some fixed temperature, T^* , which is, as a rule, the same as the melting point, T_m , established by the equality in chemical potential between the coexisting phases. The absence of superheating, $\Delta T = T^* - T_m = 0$, is ascribed [1] to the influence of the surface, that is, T^* at the surface is lower than it is in the bulk of the crystal. Melting as a phase transition of the 1st order presupposes the presence of a metastable state – a superheated crystal ($\Delta T \neq 0$). With a superheating, at least one of the above listed conditions is violated: either the crystal is placed in nonisothermal conditions or it is embedded in the matrix of another material (its surfaces are not free). The former case can occur [2] if the metal specimen is superheated by an electric current, and the latter [3] when crystallites embedded in some other material are heated. A quantity of particular interest is the limiting superheating of the crystal, which can conveniently be written in dimensionless form as $\Delta T / T_m$. Computer simulation offers a means of determining not only the relative limiting superheating but also the physical properties of the superheated crystal and the disordering mechanism. In this respect, the molecular dynamics (MD) method is unique. The introduction of periodic boundary conditions eliminates the possibility that the crystal will melt at the surface. On the other hand, the conditions of the MD experiment come very close to being adiabatic. Born's theory [4] is among the few that explain the stability of the superheated crystal. According to Born [5], the crystal fails when the shear modulus goes to zero. The manner in which the shear modulus of the cubic crystal varies with temperature is described by an expression of the form [4]

$$c_{44}^T = c_{44}^0 (1 - T/T_m)^2, \quad (1)$$

where c_{44}^0 is the shear modulus of the crystal at $T = 0$. However, in order to account for the likely superheating of the crystal, (1) should be modified by replacing T_m with the disordering temperature, T^* , of the crystal. The curve described by Eq. (1) is characterized by a rapid decrease of c_{44}^T with increasing temperature, and its curvature acquires a sign opposite to that of the experimental curve $c_{44}^T(T)$. In the molecular-dynamics model of argon (a fcc crystal), an abrupt decrease in c_{44}^T to zero has been observed at $T = T^*$ [6]. In such a case, Eq. (1) gives a poor fit to the actual behavior of c_{44}^T . As will be recalled, in terms of its structural features the bcc crystal is closer to a liquid than is the fcc crystal. For example, in the structural diffusion model [7] the radial distribution function describes the structure of the liquid better when the bcc lattice is chosen as the basis. Furthermore, for the establishment of a one-to-one correspondence between the structures of the liquid and the crystal, with the bcc lattice smaller displacements are required of the particles than is the case with the fcc crystal.

From the viewpoint of modeling, the simplest bcc solids are the alkali metals because they have a nearly spherical Fermi surface. Our choice is sodium. In the stable-state region of the sodium crystal ($T < T_m^{\text{exp}} \approx 371$ K), the elastic constants have been determined both by experiment [9, 10] and by calculation [11]. Furthermore, they have been calculated by the Monte-Carlo method [12] and by the molecular dynamics method [13]. The least accessible regions for measuring the c_{ij}^s of sodium are the low-temperature region ($0 < T < 78$ K) and the high-temperature region ($T > 371$ K, the superheated crystal). In the low-temperature region, a martensitic bcc-to-hcp transformation has been observed [14]; it proceeds as a 1st order phase transition and gives rise to a large hysteresis in the properties of the sodium crystal. In metals, superheating takes place with fast processes where the equilibrium properties of crystals are difficult to deter-

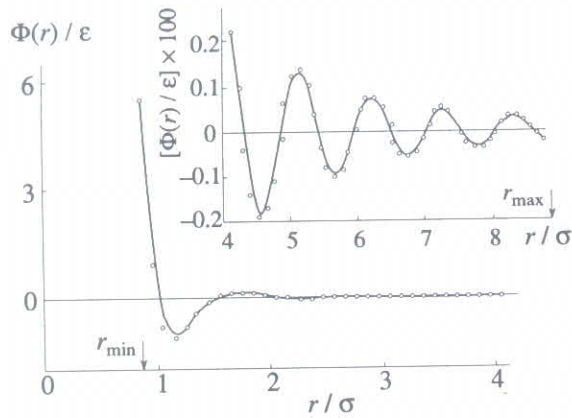


Fig. 1. Additive pair interaction potential after Schiff [16] for sodium. Potential parameters: $\sigma = 0.324$ nm, $\epsilon/k = 599$ K.

mine. Theoretical calculations [15] are complicated by the noticeable anharmonism of crystals at high temperatures and by the presence of a great number of vacancies.

The present study attempts to answer the following questions. To what extent is Born's concept of mechanical instability applicable to the bcc crystal? Which type of deformation is primarily responsible for the instability of the superheated bcc crystal? What accounts for the differences and similarities in the disordering mechanisms of the bcc and fcc crystals? What is the limit for the superheating of the bcc crystal? Additionally, we trace the response of the elastic constants of the crystal to variations in internal pressure over a wide temperature range.

CALCULATION OF THE ELASTIC PROPERTIES

The model crystal was heated stepwise, beginning from 17 K. The starting configuration was the ideal bcc lattice. The number of atoms in the basic cell was $N = 128$. The time step in integrating the equations of motion was set at $\Delta t = 2 \times 10^{-15}$ s. Every succeeding state of the system was calculated from the last configuration of the preceding state. At every next temperature, the system was first brought to equilibrium on the interval $\sim 5000\Delta t$, and the elastic properties of the crystal were usually calculated on the interval $\sim 15,000\Delta t$. The temperature was changed by scaling the velocities of the particles at every time step. The interaction of particles in the model was described by Schiff's potential [16]. The range of action of this effective pair potential (Fig. 1) is limited by the radius r_{\min} ($\Phi(r_{\min}) \approx 40kT_m$) on the left and by the maximum size of the MD cell, $r_{\max} = \sqrt{3}L$, on the right, where k is the Boltzmann constant and L is the edge of the basic cell.

For cubic crystals the conditions of thermodynamic stability can be defined as

$$T/c_p > 0 \quad c_{11}^T > 0 \quad c_{44}^T > 0 \quad c_{11}^T - c_{12}^T > 0, \quad (2)$$

where c_p is the heat capacity at constant pressure and c_{ij}^T are the isothermal second-order elastic constants.

The first inequality in Eq. (2) is the thermal stability criterion of the crystal, and the next three inequalities are related to its mechanical stability. In this paper, we are concerned solely with the mechanical stability of the sodium crystal. Isothermal compressibility is connected to the elastic constants c_{ij}^T by a relation of the form

$$\beta_T = 3 / (c_{11}^T + 2c_{12}^T). \quad (3)$$

The calculations were made on the NVE ensemble, that is, under the assumption of constancy of the number of particles N , the volume of the MD cell V , and the internal energy E . The temperature dependence of the isothermal elastic constants is represented by the quasi-isobar $p \approx 20 \pm 10$ MPa. The pressure was determined by the Clausius virial theorem

$$p = \frac{NkT}{V} - \frac{1}{3V} \sum_{i>j} r_{ij} \frac{\partial \Phi(r_{ij})}{\partial r_{ij}}. \quad (4)$$

The second-order elastic constants were calculated by the technique proposed in Ref. [17]

$$c_{ij}^T = c_{ij}^B + c_{ij}^f + \Delta c_{ij}^B + \Delta c_{ij}^a, \quad (5)$$

where c_{ij}^B and c_{ij}^f are the Born and fluctuation terms, respectively [17]. The correction for the Born term, $\Delta c_{ij}^B = c_{ij}^\infty - c_{ij}^N$, was found for a static ideal lattice, where c_{ij}^∞ is the elastic constant of an infinite lattice and c_{ij}^N is the elastic constant of a cubic lattice containing N atoms.

In order to derive the canonical ensemble average from the MD average, one needs corrections of value $\sim N^{-1}$. For the second-order elastic constants such corrections are [18]

$$\Delta c_{11}^e = \Delta c_{12}^e = \frac{NkT(\gamma c_v - 1)^2}{c_v}; \quad (6)$$

$$\Delta c_{44}^e = 0, \quad (7)$$

where γ is the Grüneisen constant and c_v is the specific heat at constant volume. The values of γ for the molecular-dynamics model of the sodium crystal are determined in Ref. [15].

The cubic crystal is characterized by six independent third-order elastic constants: c_{111}^T , c_{112}^T , c_{123}^T , c_{144}^T , c_{166}^T , and c_{456}^T (in Voigt notation). In the general form, the expression for c_{ijk}^T is written as

$$c_{ijk}^T = c_{ijk}^B + c_{ijk}^{f_1} + c_{ijk}^{f_2} + \Delta c_{ijk}^B + \Delta c_{ijk}^e. \quad (8)$$

Here, two fluctuation contributions are isolated. One can be written as $c_{ijk}^{f_1} = 1/(VkT)$ (fluctuation terms), and the other, as $c_{ijk}^{f_2} = 1/(V(kT)^2)$ (fluctuation terms). The Born term c_{ijk}^B and its correction, Δc_{ijk}^B , are the same as the corresponding contributions to the second-order elastic constants, whereas the ensemble correction, Δc_{ijk}^e , is given, according to Ref. [6], by

$$\Delta c_{ijk}^e = -\frac{\langle (T - \langle T \rangle)^2 \rangle^{1/2}}{\langle T \rangle} (c_{ijk}^f + c_{ijk}^f), \quad (9)$$

where the French quotes, $\langle \dots \rangle$, designate a time average. The equations for the calculation of the Born and fluctuation contributions to c_{ijk}^T are even more unwieldy than for the corresponding terms of c_{ij}^T [6]; accordingly, we leave them out here. Note only that the contributions c_{ijk}^B , c_{ijk}^f and c_{ijk}^f contain the sums of the first, second and third-order derivatives of the interatomic interaction potential.

The pressure derivatives of c_{ij}^T , of the shear modulus $s^T = (c_{11}^T - c_{12}^T)/2$, and of the isothermal bulk modulus $B^T = \beta_T^{-1}$ are given by Refs. [19, 20]

$$\begin{aligned} \frac{dc_{11}^T}{dp} &= -(2c_{11}^T + 2c_{12}^T + c_{111}^T + 2c_{112}^T) / (3B^T); \\ \frac{dc_{12}^T}{dp} &= -(-c_{11}^T - c_{12}^T + c_{123}^T + 2c_{112}^T) / (3B^T); \\ \frac{dc_{44}^T}{dp} &= -(c_{11}^T + 2c_{12}^T + c_{44}^T + c_{144}^T + 2c_{166}^T) / (3B^T); \\ \frac{ds^T}{dp} &= -(3c_{11}^T + 3c_{12}^T + c_{111}^T - c_{123}^T) / (6B^T); \\ \frac{dB^T}{dp} &= -(c_{111}^T + 6c_{112}^T + 2c_{123}^T) / (9B^T). \end{aligned} \quad (10)$$

The third-order elastic constants play an important role in solid-state physics. They can be used [21] to construct the interatomic interaction pair potential. To a first approximation, these constants allow the calculation of the anharmonic terms of the interaction potential and the generalized Grüneisen constant. The moduli c_{ijk}^T are used in the stability analysis of heavily strained lattices. Note that from ultrasonic measurements one can determine the mixed [22] (adiabatic-isothermal) constants c_{ijk} . In order to calculate the isothermal elastic constants c_{ijk}^T by resort to c_{ijk} , one must know the heat capacity at constant volume c_V and the derivatives $\partial c_{ij}^e / \partial T$.

RESULTS

The melting point in the model has been found from the break point (Fig. 2) in the potential energy versus temperature curve. The value thus found, $T_m = 423$ K, is higher than the melting point found by a physical experiment (≈ 371 K) and in the MD model of sodium [23] (≈ 396 K), with a pseudopotential dependent on the density of the electron gas. The rms displacement of particles at T_m has been found to be 24% of the lattice constant, which agrees with the Lindemann criterion [1]. The internal energy increases with temperature more quickly at $T > T_m$ than at the lower values of T . The last two calculations ($T = 460$ K and $T = 470$ K) were made beginning from the last configuration corresponding to

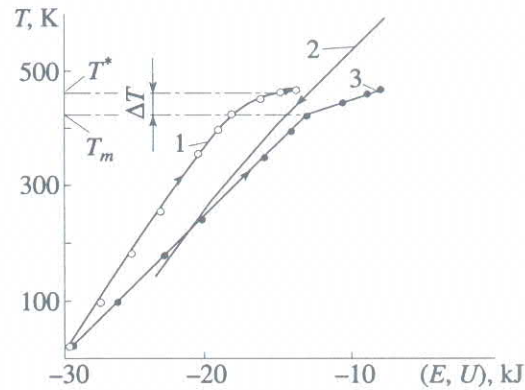


Fig. 2. Temperature variations of the bcc crystal on heating and on failure and on cooling: $T(E)$ of the crystal (1), $T(E)$ of the liquid (2), $T(U)$ of the crystal (3). Here E is the internal energy of crystal, and U is its potential energy.

$T = 453$ K. In the second calculation a state described by the liquid branch was all but reached (curve 2 in Fig. 2). Below T_m , curve 2 characterizes a supercooled liquid.

The time required to calculate the elastic properties of the crystal increases with increasing temperature. The worst convergence of c_{ij}^T and c_{ijk}^T is in the failure region of the crystal. An irreversible structural rearrangement in the sodium crystal occurs at $T \approx 460$ K, that is, at a relative superheating of $(T^* - T_m) / T_m \approx 0.09\%$. The elastic constants c_{ijk}^T converge more slowly than do c_{ij}^T . Slowly damped fluctuations at large time intervals, leading to a considerable ($\sim 30\%$) statistical error, were observed only for c_{123}^T and c_{166}^T . The error in determining the elastic constants c_{ij}^T does not exceed 5% even at $T > 453$ K.

The temperature dependence of the second-order elastic constants, which characterize the stability of the crystal, is illustrated in Fig. 3. In the low-temperature region ($T < 70$ K), the modulus $s^T = (c_{11}^T - c_{12}^T)/2$ goes to zero; a likely martensitic transformation in the sodium crystal is thus predictable. In the crystal-liquid transition region, the first modulus to go to zero is likewise the modulus s^T , followed by c_{44}^T . The modulus s^T characterizes the shear deformation in the (110) plane which, in the bcc lattice, is most populated. Note that in the fcc lattice the (111) plane is the most populated. The modulus μ^T , which characterizes the slip of particles in that plane, is the first to go to zero [24] upon the failure of the fcc argon crystal. For the bcc sodium crystal, the elastic constant c_{11}^T , which is related to uniaxial tension in the $\{100\}$ direction, remains nonzero at T^* .

Among the third-order elastic constants, only c_{123}^T and c_{166}^T undergo great change at $T < 100$ K (Fig. 4). However, as the crystal approaches the disordering temperature, the change is most noticeable in c_{111}^T and c_{112}^T . The behavior of $c_{ijk}^T(T)$ does not characterize the stability of the crystal directly. However, the constants c_{ijk}^T , when taken together with c_{ij}^T , do reflect the behavior of the pressure derivatives of the elastic constants (10). In the model, no rapid changes were observed in any of the five derivatives $(dc_{11}^T/dp, dc_{12}^T/dp, dc_{44}^T/dp, ds^T/dp, and$

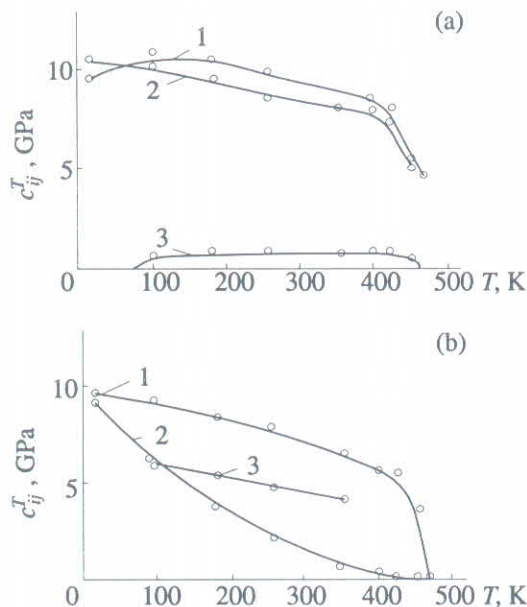


Fig. 3. Second-order elastic constants of the crystalline solid. (a): c_{11}^T (1); B^T (2); s^T (3). (b): c_{44}^T (MD calculation in the present paper) (1); calculation by Eq. (1) (2); experiment [10] (3).

dB^T/dp) for the sodium crystal up to T_m (Fig. 5); but changes do rise abruptly when the disordering temperature T^* is approached. The second-order constants c_{ij}^T , as well as s^T and B^T , decrease most significantly in the temperature range from 423 K to 460 K (Fig. 3). A superheated crystal with an impaired elasticity responds more strongly to changes in pressure than does a stable crystal. As soon as the deformation caused by the thermal motion of atoms in the crystal becomes irreversible ($T = 470$ K), a fall occurs in the derivatives dc_{ij}^T/dp , ds^T/dp , and dB^T/dp .

DISCUSSION

As the present study shows, only a slight difference exists between the elastic constants c_{11}^T and c_{12}^T of the sodium crystal. Notably, at $\sim 0.8T_m$ the shear modulus is $s^T = (c_{11}^T - c_{12}^T)/2 \approx 0.6$ GPa. The experimental value of this modulus, as reported in Ref. [9], is $s^T = 0.611$ GPa. The low value of s^T implies that the internal stress in a solid alkali metal does not markedly differ from the hydrostatic pressure characteristic of a liquid. However, alkali-metal crystals retain appreciable shear stresses that cannot exist in a liquid. The marked difference between the calculated and experimental values of c_{44}^T is ascribed in Ref. [13] to the fact that the second-order elasticity theory does not give a faithful description of the resistance to shear in the (100) plane. The resort in Ref. [13] to the pair potential, which explicitly depends on the volume of the system, does not rectify the situation. Whereas resort to the pair potential proves effective in accounting for three- and four-body interactions in the case of the fcc lattice [25], it is not effective in the case of the bcc lattice. In order to determine

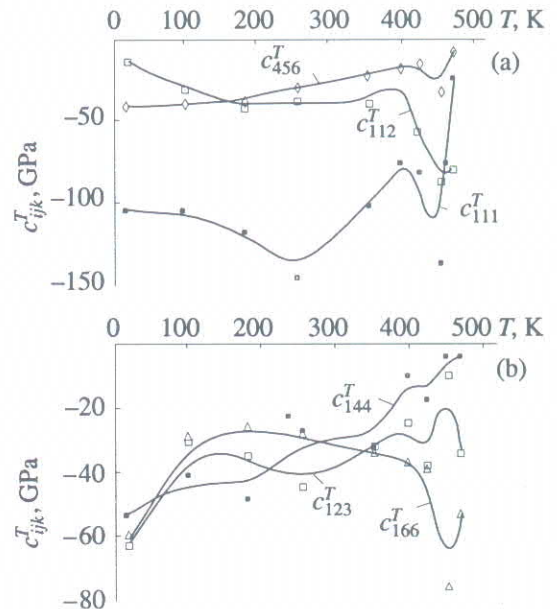


Fig. 4. Third-order elastic constants for crystalline sodium.

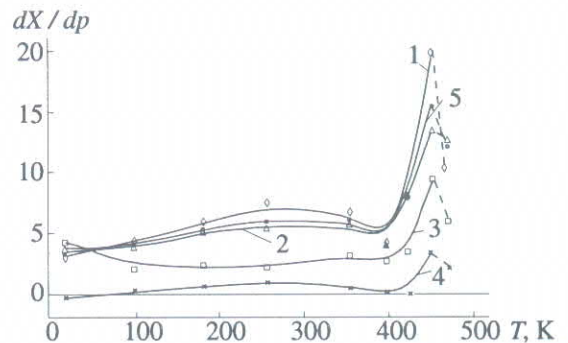


Fig. 5. Pressure derivatives of the second-order elastic constants: dc_{11}^T/dp (1); dc_{12}^T/dp (2); dc_{44}^T/dp (3); ds^T/dp (4); dB^T/dp (5). The dashed line indicates the portions corresponding to irreversible deformation in the crystal.

the elastic constant c_{44}^T more accurately, one would need to consider many-body interactions. Estimation of the relative superheating for solid metals by various experimental techniques yields $\Delta T/T_m < 0.2$.

Born's concept of mechanical instability may be extended to the bcc crystal. The instability point for the bcc crystal is determined by the shear modulus s^T , which is the first to go to zero at the disordering temperature T^* . The next to do so is the other shear modulus, c_{44}^T . The elastic constant c_{11}^T retains a finite, nonzero value at T^* . In the dynamic model, the failure of the crystal is caused by shear instability. This concept of Born's is not a generally accepted one. The result obtained by the correlated unsymmetrized method of a self-consistent field [26] suggests a different mechanism for the failure of the crystal: the first to go to zero is the bulk modulus B^T .

CONCLUSIONS

The results of the present study and those reported in Ref. [24] indicate that for cubic crystals of simple substances the critical deformation is that one associated with the slip of particles in the most populated crystallographic plane. For the bcc crystal, this is the (110) plane, and for the fcc crystal, the (111) plane. In both cases, the elastic constants rapidly decrease to zero in a narrow temperature interval. The maximum superheating for the bcc crystal (sodium) is $\sim 0.09T_m$, and for the fcc crystal (argon) [6] at $p \sim 30$ MPa, it is approximately $0.25T_m$. As is shown in Ref. [27], the presence of point defects in the crystal does not affect its superheating, which means that the superheating, ΔT , is practically identical for an initially perfect and an initially imperfect crystal. The pressure derivatives of the second-order elastic constants increase abruptly on approaching T^* . The decrease in these derivatives with increasing temperatures indicates that the structural rearrangement taking place in the crystal is irreversible in character. The position taken up by the sharp peak on the dX/dp versus T curve, where $X = c_{ij}^T, s^T, B^T$ corresponds to the disordering temperature, T^* , of the crystal, as determined when the shear moduli go to zero.

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