# Plastic deformation of solidified inert gases

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Some features of plastic deformation of solidified Ne, Ar, Kr, and Xe under plastic flow condtions are considered. It is shown that over a broad temperature range the dependence of the plastic deformation rate of crystals on temperature can be represented in the form of the law of corresponding states. The role of quantum effects is discussed.

One of the features of the plastic deformation of crystals in the region of sufficiently high temperatures and low deformation rates is the transition to a state of plastic flow,[1] in which the deformation of the test samples occurring at some constant temperature and velocity v takes place without any appreciable increase in stress. From the microscopic point of view the existence of this transition is due to the increase with increasing temperature of the probability that dislocations will overcome the local high-energy barriers which arise in the crystal as the result of the mutual blocking of dislocations in the period of hardening of the crystal[2] which precedes plastic flow.

In the case of the solidified inert gases[3-4] for a given deformation rate the transition to plastic flow with increasing temperature occurs so abruptly that in plots of the hardening it is possible to establish some arbitrary transition temperature $T_c$. Experiments show that near $T_c$ there is also a substantial change in the nature of the temperature dependence of the yield point, the elastic limit, and the relative elongation of the test samples.

For $T < T_c$ the deformation process is terminated by brittle fracture of the crystals, which according to current ideas[5] is the result of continuous accumulation of dislocations in front of a barrier, leading to formation of microcracks. It is therefore natural to define $T_c$ as the lower limiting temperature at which equality is achieved of the rates of supply and detachment of dislocations from local high-energy barriers which control the plastic deformation. Here the two rates are obviously proportional to the crystal deformation rate.

Table I shows the temperatures $T_c$ found[3,6] for two rates ($v_1 = 5.5 \times 10^{-3}$ sec$^{-1}$, $v_2 = 5.5 \times 10^{-4}$ sec$^{-1}$) of uniaxial stretching of polycrystalline samples of Ne, Ar, Kr, and Xe. Since the ratios of $T_c$ to the melting temperatures of the crystals drop appreciably in going from Xe to Ne, the suggestion was made that this is due to a dependence of the $T_c$ values on the quantum parameter[7] $\lambda = h/r_0(m\epsilon)^{1/2}$ (m is the mass of the atom, $r_0$ and $\epsilon$ are the parameters of the Lennard-Jones potential), which characterizes the degree of influence of zero-point lattice vibrations on the properties of a solid. Since $\lambda$ is a function of the ratio of the zero-point mean-square deviations of the atoms $\Delta_0^2$ to $r_0^2$ (to a first approximation $\lambda \sim \Delta_0^2/r_0^2$; see ref. 8), it was desirable to compare the mean-square deviations for Ne, Ar, Kr, and Xe which correspond to the $T_c$ values obtained.

TABLE I. Temperatures $T_c$ of solid Ne, Ar, Kr, and Xe

| Gas | $T_c$, °K |  | $T_c/T_{m.p.}$ |  |
|---|---|---|---|---|
|  | $v_1$ | $v_2$ | $v_1$ | $v_2$ |
| Ne | 14.5 | 10.5 | 0.59 | 0.43 |
| Ar | 65 | 56 | 0.77 | 0.66 |
| Kr | 90 | 78 | 0.78 | 0.67 |
| Xe | — | 115 | — | 0.72 |

Figure 1 shows $\Delta^2/r_0^2$ as a function of the temperature, calculated from 0°K to $T_{m.p.}$ according to Peresada's method[9,10] with use of the characteristic temperatures $\Theta_P$ (Table II).

It is easy to see that, like the melting point, the transition of solid Ar, Kr, and Xe to plastic flow occurs approximately at the same level of mean-square deviation, determined by the rate of stretching. The deviation from Lindeman's law in the case of Ne is evidently due to the substantial influence of quantum effects.[11] We are struck, however, by the fact that the nature of this influence on the melting point and on the transition to plastic flow turns out to be quite similar. As a result, for a given rate of stretching the ratios of the mean-square deviations corresponding to temperatures $T_c$ to the mean-square deviations at the melting points are identical for all four crystals (Fig. 2). The dot-dash straight lines drawn through the experimental values of $T_c$ are upper limits of brittleness of the crystals corresponding to rates $v_1$ and $v_2$. For small deformation rates the crystals may not reveal their typical brittleness properties down to absolute zero temperature, which is due to the possibility that dislocations may acquire the kinetic energy necessary to surmount the barriers not only as the result of thermal fluctuations but also of quantum fluctuations.[12]

An analysis carried out permits the suggestion that over a wide range of temperatures the rate of plastic deformation of the group of crystals studied can be represented in the form of the law of corresponding states

$$v = f(\Delta^2/\Delta^2_{m.p.}), \tag{1}$$

which can be considered a generalization for the case of nonzero temperatures of Bernardes' quantum-mechanical law of corresponding states for the properties of Van der Waals crystals.[8] It is easy to show that in the region of sufficiently high temperatures it goes over naturally into the classical de Boer relation[7]:

$$v = \varphi(kT/\varepsilon). \tag{2}$$

Strictly speaking, the velocity v in Eqs. (1) and (2) should be reduced by the velocity $(\epsilon/m)^{1/2}$ characteristic of the crystal. In view of the small difference in the values of the latter (Table II) and the strong exponential dependence of v on $\Delta^2/\Delta^2_{m.p.}$ (see below), the

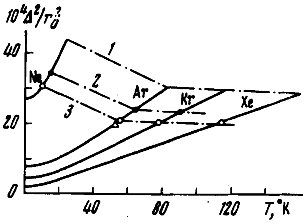

FIG. 1. Temperature dependence of the mean square deviations of solidified Ne, Ar, Kr, and Xe: ○ – $v_1$ = 5.5 × $10^{-3}$ sec$^{-1}$, ○ – $v_2$ = 5.5 × $10^{-4}$ sec$^{-1}$, Δ – $v_3$ = 3.3 × $10^{-4}$ sec$^{-1}$. 1 – line of melting points of the crystals, 2 – line of temperature $T_c$ corresponding to the rate $v_1$, 3 – line of temperature $T_c$ corresponding to the rate $v_2$.

TABLE II. Parameter values used.

| Gas | $\varepsilon\cdot10^{16}$, c | $r_0$, Å | $(\varepsilon/m)^{1/2}\cdot10^{-4}$, cm/sec | $\Theta_P$, °K | $\Theta_D$, °K | $T_{m.p.}$, °K | $\lambda$ | $C$ |
|---|---|---|---|---|---|---|---|---|
| Ne | 50.6 | 3.131 | 1.22 | 72.5 | 74 | 24.48 | 0.510 | (2.50) |
| Ar | 165 | 3.820 | 1.57 | 89.5 | 93.3 | 83.75 | 0.165 | (3.74) |
| Kr | 227 | 4.084 | 1.27 | 69.9 | 72 | 116.55 | 0.091 | (3.88) |
| Xe | 319 | 4.446 | 1.20 | 61 | 65 | 161.35 | 0.0056 | 3.90 |

need of this normalization loses its meaning for the crystals considered.

In Fig. 3 for $T \geq T_c$ ($v = 5.5 \times 10^{-4}$ sec$^{-1}$) we have shown the arbitrary tensile strength reduced by the molecular parameters $\sigma_b^* = \sigma_b r_0^3/\epsilon$ of solidified Ne, Ar, Kr, and Xe as a function of $\Delta^2/\Delta^2_{m.p.}$. It is easy to see that under plastic flow conditions a given deformation rate (for $T = T_c$ this rate is the maximum possible) is achieved at a certain reduced stress which is the same for all crystals.

The existence of a rather clear dependence of v and $\sigma_b^*$ on $\Delta^2/\Delta^2_{m.p.}$ for solidified Ne, Ar, Kr, and Xe leads to the one conclusion that, under conditions of stationary plastic flow, both the limiting value of deformation rate and the stress necessary to maintain a given value of it are insensitive to the structural state of the crystal and are determined only by its thermodynamic state.

We turn now to the question of the nature of the dependence of v on $\Delta^2/\Delta^2_{m.p.}$. Since in the high temperature region $\Delta^2 \sim T$ and a classical thermal activation function is valid for the rate v,

$$v \sim \exp(-U/kT), \tag{3}$$

we reach the conclusion that

$$v \sim \exp(-a^2\Delta^2_{m.p.}/\Delta^2), \tag{4}$$

where the dimensionless parameter $a^2$ characterizes the effective height U of the barrier preventing motion of dislocations in the crystal. Writing $a^2$ in the form of the ratio $\Delta^2/2\Delta^2_{m.p.}$, we obtain for the deformation rate

$$v \sim \exp(-\delta^2/2\Delta^2),$$

i.e., under conditions of stationary flow the plastic deformation rate of solidified inert gases is proportional, to the accuracy of the pre-exponential factor, to a Gaussian probability for the amplitude δ of the quantum oscillator. In the model considered it is easy to show that δ is connected with the barrier height by the relation

$$U^* = CG^*\delta^{2*}. \tag{5}$$

Here

$$U^* = U/\varepsilon, \quad G^* = Gr_0^3/\varepsilon, \quad \delta^{2*} = \delta^2/r_0^2,$$

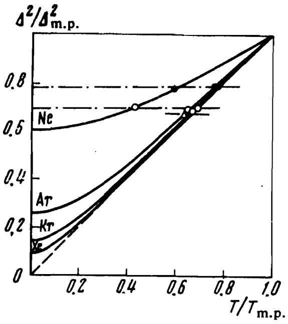

FIG. 2.

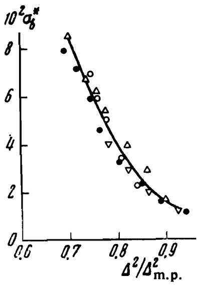

FIG. 3.

FIG. 2. Mean square deviations of solidified Ne, Ar, Kr, and Xe in reduced coordinates as a function of temperature. The dashed straight lines show the dependence for a classical crystal, ○ – $v_1$ = 5.5 × $10^{-3}$ sec$^{-1}$, ○ – $v_2$ = 5.5 × $10^{-4}$ sec$^{-1}$, Δ – $v_3$ = 3.3 × $10^{-4}$ sec$^{-1}$.

FIG. 3. Tensile strength reduced by the molecular parameters $\sigma_b^* = \sigma_b r_0^3/\epsilon$ as a function of the reduced mean square displacements (v = 5.5 × $10^{-4}$ sec$^{-1}$). ○ – Ne, ∇ – Ar, Δ – Kr, ○ – Xe.

G is the elastic modulus, and C is a coefficient of proportionality determined by the nature of the interaction and consequently the same for all four crystals. When Eq. (5) is taken into account the deformation rate is

$$v \sim \exp\left(-\frac{1}{2C}\frac{U^*}{G^*}\frac{1}{\Delta^{2*}}\right). \tag{6}$$

Comparing (6) and (3) in the region of sufficiently high temperatures, we find that

$$C = T^*/2G^*\Delta^{2*}, \quad T^* = kT/\varepsilon. \tag{7}$$

The constant C can be determined with a very small error from $T^*$, $G^*$, and $\Delta^{2*}$, referred to the melting point of solid Xe. Calculations in which $G^*$ was taken as the value of the reduced shear modulus obtained from ultrasonic measurements[13] give a C value of 3.90 for Xe (Table II). The results of similar calculations for solidified Ne, Ar, and Kr, while not very correct, are shown in Table II in parentheses.

From the data on two rates v and the corresponding values of $\Delta^{2*}$ it is now easy to evaluate the effective height of the barriers which prevent motion of dislocations in the crystals. The calculations show that for all solidified inert gases the barrier height is of the order of the crystal binding energy. The substantial value of the activation energy of the process indicates that in plastic flow the probability of unpinning dislocations from obstacles is apparently determined by the rate of diffusion processes.[14]

If quantum effects on the properties of crystals at melting can be neglected, and if we use the expression for C at $T = T_{m.p.}$, it is convenient to represent Eq. (6) in the form

$$v \sim \exp\left(-\frac{U^+}{G^+}\frac{1}{\Delta^{2+}}\right), \tag{8}$$

where $U^+ = U/kT_{m.p.}$, $G^+ = G/G_{m.p.}$, $\Delta^2/\Delta^2_{m.p.}$. Use of this dependence is obviously justified only in the case of solidified Ar, Kr, and Xe.

The reduced mean-square deviations used in Eqs. (6) and (8) can conveniently be considered as certain effective temperatures $T_{eff}$. Thus, we have

$$v \sim \exp(-U/kT_{eff}), \tag{9}$$

where in Eq. (8) $T_{eff}$ has the form

$$T_{eff} = T_{m.p.}\frac{G}{G_{m.p.}}\frac{\Delta^2}{\Delta^2_{m.p.}}.$$

In the region of high temperatures $T_{\text{eff}} = T$. Near 0°K, using the well known Debye expression[15] for $\Delta^2$, it is easy to show that

$$T_{\text{eff}} = \frac{G_0}{G_{\text{m.p.}}} \frac{\Theta_D}{4} \left[ 1 + A \left( \frac{T}{\Theta_D} \right)^2 \right], \tag{10}$$

where $\Theta_D$ is the characteristic Debye temperature, $G_0$ is the elastic modulus at 0°K, and the constant $A = 2\pi^2/3$. This discussion naturally assumes that the same plastic deformation mechanism is retained down to absolute zero temperature.

At absolute zero temperature the maximum plastic deformation rate permitted is determined only by the value of the zero-point mean-square deviations of the atomic particles. For quantum crystals, in view of the substantial atomic mobility, $v$ can reach a very high value. Here in the first approximation

$$v \sim \exp(-c/\lambda), \quad c = \text{const}, \tag{11}$$

which essentially agrees with the expression for quantum tunneling of particles through a high-energy barrier.[16]

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196