THE DEPENDENCE OF MICROHARDNESS AND YIELD STRESS ON THE TETRAGONALITY OF POINT DEFECTS IN IONIC CRYSTALS WITH CUBIC SYMMETRY

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According to experiments, cubic crystals often contain defects of tetragonal symmetry. For instance, after irradiating f.c.c. metals by electrons or neutrons a great number of interstitials emerge which bring about tetragonal deformation of the lattice [1]. In b.c.c. metals, interstitials C, N and O also tetragonally deform the lattice. In alkali-halides such as NaCl and KCl divalent cations like Ca^{2+} are often present at the cation sites and generally form complexes (dipoles) made of an impurity ion and a cation vacancy associated with it [2]. These complexes also cause tetragonal distortion of the crystal lattice. NABARRO [3] and FLEISCHER [4] have proved that in cubic lattices the tetragonal point defects strongly interact with the dislocations, and by this means have an influence on the yield stress. The increment of yield stress due to this interaction is given by [5]:

$$\Delta\tau^d = 1.48 \cdot \mu \cdot \Delta\lambda^* \cdot N_d \tag{1}$$

where $\mu = 1/2\,(C_{11} - C_{22})$ is the shear modulus, C_{ij} are the elastic moduli, $\Delta\lambda^*$ is the so-called dipole strength that characterizes the lattice-deforming effect of the dipoles and N_d is the concentration of the dipoles. The aim of the present paper is to determine the value of $\Delta\lambda^*$ for NaCl containing different kinds of impurities.

According to (1) $\Delta\lambda^*$ can be obtained by measuring the increment of the yield stress; it is, however, easier to determine it by the utilization of microhardness measurements. Since according to our measurements there exists a linear relation between the microhardness increment ΔH and the yield stress increment $\Delta\tau$ (Fig. 1) microhardness measurements were applied. In an earlier paper [6] it was pointed out that in NaCl:Ca^{2+} crystals with not too high impurity concentration the microhardness increments caused by Ca^{2+} impurities can be attributed to two factors. One reason is the presence of elastic dipoles, the other one is the electric charge on the dislocations. Denoting the corresponding terms by H^d and H^q, and considering the proportionality

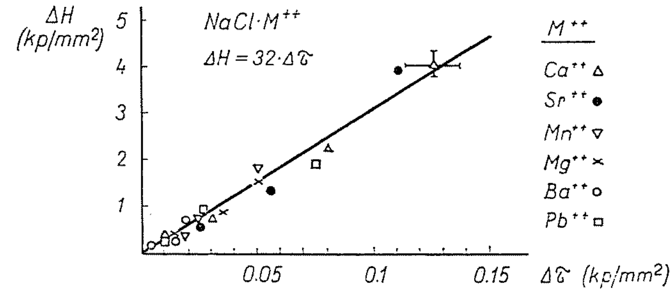

Fig. 1. The correlation between microhardness increment ΔH and yield stress increment $\Delta\tau$ for NaCl crystals containing various kind of divalent cation impurities

between the charges and the concentration of free cation vacancies (N_v) [7], the above mentioned results may be written in the following form:

$$\Delta H = H - H^\circ = H^q + H^a = A \cdot N_v^2 + B \cdot N_d \tag{2}$$

where H and H° are hardnesses of a contaminated sample, and of a pure crystal (concentration of any kind of impurity less than 10^{-7} mol/mol), respectively A and B are constants given by determining ΔH for various values of N_v and N_d. N_v and N_d can be modified by varying the impurity concentration (c). The measurements for various types of impurities gave the results presented in Fig. 2.

The constants A and B for various types of impurities can be determined from the relationships between c, N_v and N_d and the curves in Fig. 2.

Using Eq. (1) and taking the proportionality between ΔH and $\Delta\tau$ into account:

$$\Delta\lambda^* = \frac{B}{43.36 \cdot \mu}. \tag{3}$$

So $\Delta\lambda^*$ is easy to calculate from constant B obtained in microhardness measurements. As it is expected, $\Delta\lambda^*$ has different values for different impurities, namely they cause different distortions of the crystal lattice. It is obvious to suppose that the value $\Delta\lambda^*$ depends on the ionic radius of the impurity. This dependence is, however, against expectations, not monotonous but has a maximum for Sr^{2+} impurity (Fig. 3). To find out the physical reason for the existence of the maximum it seems reasonable to calculate the strain field around a dipole using atomistic model. Such investigations are in progress.

Note that our $\Delta\lambda^*$ values are lower than those published by others, since the contribution of charged dislocations to the yield stress is usually ignored, although in a number of cases this contribution is of the same order of magnitude than that of the dipoles.

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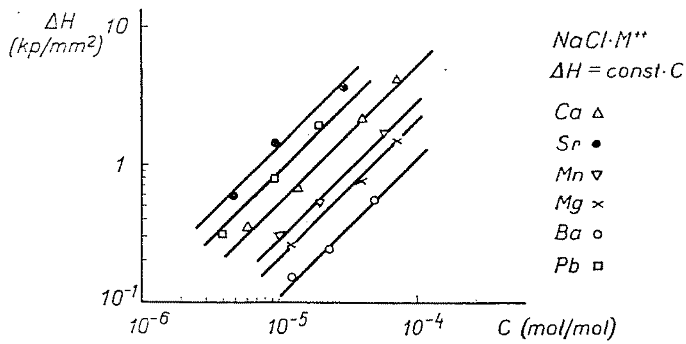

Fig. 2. The dependence of microhardness increment on the impurity concentration for various kind of impurities

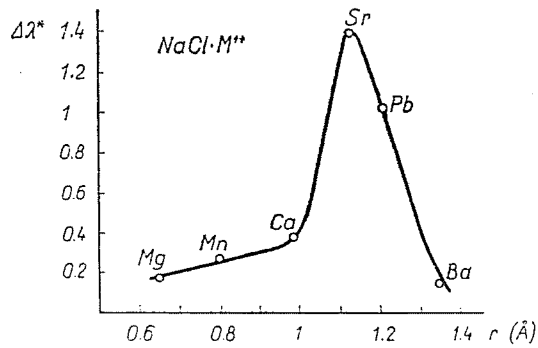

Fig. 3. The relation between dipole strength $\Delta\lambda^*$ and the ionic radius of the dipole forming impurity

Summary

The effect of various kinds of impurities on the yield stress of NaCl crystals has been investigated. The tetragonality of point defects caused by impurities is calculated from the variation of the yield stress and it is pointed out that its dependence on the ionic radius of the impurities is other than monotonous.

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