Correlation of the Peierls Stresses with Crystal Structures Based on a Generalized Peierls-Nabarro Model

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The Peierls stress τ_P, which is one of the most fundamental quantities describing the plastic behaviors of crystalline solids, is the minimum external shear stress necessary for a dislocation to overcome the potential barrier arising from the lattice periodicity without any assistance of thermal or quantum lattice vibration. Most theoretical studies on the Peierls stress of dislocations in crystals is based on the Peierls-Nabarro (PN) dislocation model, where only two lattice planes facing the glide plane are treated as discrete lattice and the two half infinite crystals above and below the planes are approximated as elastic continuum. The formula, obtained by Peierls and Nabarro[1,2] and revised by Huntington[3] assuming the sinusoidal shear interaction between atomic rows in the two planes, is $\tau_P/G = C\exp(Ah/b)$ with $A=\pi/(1-\nu)$ and $C=1/(1-\nu)$, where G is the shear modulus, ν the Poisson ratio, h the glide plane spacing and b the magnitude of the Burgers vector. This formula connects the parameters describing the crystal structure to the value of τ_P. Ohsawa et al.[4] computed self-consistently the equilibrium configuration of the PN dislocation assuming the longer-range inter-atomic-row potentials instead of the sinusoidal one, and showed that the above formula is satisfied approximately but with different A and C values depending on the shape of the interaction potential.

The PN model and its formulation have so far been described in literatures mainly for the edge dislocation in the lattice with the periodicity b in the direction of dislocation motion. However, in many real crystals, it is known that non-edge dislocation controls the deformation and the periodicity is not same as b. Hence, in order to compare experimentally estimated τ_P's with the PN models, it is necessary to generalize the PN formula for dislocations with a variety of characters. In the generalization, b in the original formula should be replaced by lattice periodicity δ in the direction of the dislocation motion. The factors A and C were obtained to be $A=\pi/(1-\nu)$ and $C=1/(1-\nu)$ for edge dislocation and $A=\pi$ and $C=1$ for screw dislocation. A and C for mixed dislocations should be given as the conventional weighted averages of the factors for screw and edge dislocations, i.e. $A=\pi[\sin\theta/(1-\nu)+\cos\theta]$ and $C=A/\pi$ where θ is the angle between the Burgers vector and the direction of the dislocation. Using these factors, the generalized formula of the PN relation is expressed as $\tau_P/(GC) = \exp(Ah/\delta)$.

Because the value of τ_P corresponds to the critical resolved shear stress τ_c at the absolute zero, we could obtain it by extrapolating the temperature T dependence of τ_c directly to the absolute zero in the case of metallic and some ionic crystals for which τ_c vs. T relations are available down to low enough temperatures. However, for materials like covalent crystals and intermetallic compounds, τ_c's have not been measured at sufficiently low T because of the brittleness at low temperatures. We have estimated τ_P's for such brittle materials by a method based on the line tension model of the kink-pair

formation enthalpy. By this method τ_P is given as $(mk_BT_0)^2/(d^3b\kappa)$, where m is a constant around 30, k_B the Boltzmann's constant, T_0 the temperature at which the T-dependence of τ_c vanishes, d the period of the potential called the Peierls potential which a dislocation feels, and κ the line tension of the dislocation. The value of κ for each crystal can be numerically computed by use of the elastic constants. Despite some ambiguity of m and T_0, τ_P's could be estimated with an accuracy.

τ_P's of dislocations of 66 slip systems in 52 crystals have been estimated experimentally either by direct extrapolation of the τ_c vs. T curve to 0 K or by the line-tension approach. τ_P/G values are distributed over four orders of magnitude, 10^{-5} to 10^{-1}, but those for a group of crystals with the same crystal structure are within an order of magnitude. In order to see the correlation between τ_P's and the crystal structure, we plot $\tau_P/(GC)$ against Ah/δ in FIG. 1, based on the generalized PN model mentioned above. Generally τ_P's are lower than the theoretical relations of Huntington (H) and Ohsawa et al. (O$_i$) This can be explained partially by the fact that only an incomplete relaxation of dislocation core is taken into consideration in the model. However, the large deviations of about two orders of magnitude at $Ah/\delta \sim 5$ cannot be attributed solely to it, and some other factors should be involved. In the plot, there is a tendency that τ_P's become higher as the covalent bonding character increases, reflecting the general tendency of the normalized theoretical shear strength of crystals [5].

References
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FIG. 1. Generalized PN plot of the estimated τ_P. Lines denoted as H and O$_i$ are the theoretical relations of Huntington [3] and Osawa et al.[4], respectively.