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Correlation of Peierls-Nabarro Stress with Crystal Structure

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According to the theory of Peierls and Nabarro[1], the Peierls-Nabarro stress τ_p is given by

$$\tau_p \sim \frac{2G}{1-\nu} \exp\left(-\frac{2\pi}{1-\nu} \frac{h}{b}\right), \quad (1)$$

where h is the natural spacing of atomic planes parallel to slip plane, b the magnitude of Burgers vector, G the shear modulus and ν the Poisson's ratio.

In Fig. 1. are shown the experimental values of τ_p/G against h/b . The τ_p of b.c.c. metals (K[2], Fe, Nb, Ta[3], Mo[4]) and a B2 compound β -CuZn[3], and those for $\{110\}\langle 1\bar{1}0\rangle$ slip in ionic crystals of NaCl-type (LiF, NaCl, KCl etc.[5-7]) were determined accurately by the plastic deformation at low temperatures ($T \approx 0K$). To be noted is that h/b for β -CuZn is a half of that for b.c.c. metals because $b = a\langle 111\rangle$. When it is difficult to deform crystals at low temperatures, τ_p is deduced by an appropriate extrapolation to $0K$ of the c.r.s.s. The τ_p for $\{001\}\langle 110\rangle$ slip in ionic crystals of NaCl-type[6,7] and those for zinc blende structure (CdTe, HgSe, CuCl, and CuBr[8]), and of b.c.c.³He [9] were estimated in this way. The h/b for zinc blende structure is 0.614 when dislocations move between shuffle set and 0.204 between glide set. An f.c.c. metal Ag[10], alkali-halides of CsCl-type (CsBr and CsI, $\{110\}\langle 001\rangle$ slip) [11,12] and PbS ($\{001\}\langle 110\rangle$ slip) [7] are easy to deform at low temperatures, but one can find no region of Peierls mechanism. In these cases the c.r.s.s. at $T \approx 0K$ gives only an upper limit of τ_p . A crude estimate of τ_p for basal slip in α -Al₂O₃ is possible from the data of c.r.s.s. at 1200-1500°C [13]. The plasticity data of α -quartz under hydrostatic pressure at 300-1000°C [14] indicate that τ_p of α -quartz should be several GPa. For α -Al₂O₃ and α -quartz, h/b is assumed to be the widest spacing of atomic planes normal to c-axis.

The solid lines in Fig. 1 are the relations of eq.(1) for $\nu=0.3$. The line A is the case of perfect (non-splitting) dislocations. Some of the experimental τ_p/G are close to the line A, but the others are far below it. When dislocations split into partial dislocations, b in eq.(1) is replaced by b^* of the partials. The line B is the case of $b^*=b/2$ and the line C is for $b^*=b/\sqrt{3}$ (Shockley partials in f.c.c. lattice). The splitting of dislocations in f.c.c. metals and β -CuZn is well known. Dislocations in CsBr and CsI can also split ($b^*=b/2$) because of the low stacking fault energy [12]. Fig. 1 suggests the splitting of $\{110\}\langle 110\rangle$ dislocations in ionic crystals of NaCl-type and $\{001\}\langle 110\rangle$ dislocations in PbS.

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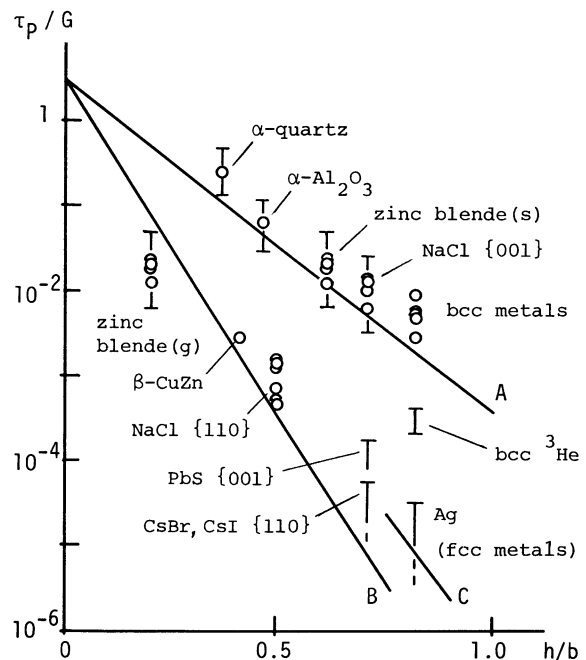


Fig. 1. τ_p vs h/b . Solid lines indicate the relations of eq.(1) for $\nu=0.3$. A: for perfect dislocations with Burgers vector b ; B: for half dislocations with $b^*=b/2$, and C: for Shockley partials in f.c.c. lattice with $b^*=b/\sqrt{3}$. (s) and (g) for zinc blende structure denote shuffle set and glide set, respectively.