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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 $\sigma_p$ is given by

$$\sigma_p \approx \frac{2G}{1-v} \exp\left(-\frac{2\pi h}{1-v}b\right),$$

(1)

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

In Fig. 1 are shown the experimental values of $\sigma_p/G$ against $h/b$. The $\sigma_p$ of b.c.c. metals (K[2], Fe, Nb, Ta[3], Mo[4]) and a B2 compound $\beta$-CuZn[3], and those for $\langle 110\rangle \{110\}$ slip in ionic crystals of NaCl-type (LiF, NaCl, KCl etc.[5-7]) were determined accurately by the plastic deformation at low temperatures ($T=0K$). To be noted is that $h/b$ for $\beta$-CuZn is a half of that for b.c.c. metals because $b=\alpha l_{\perp}$. When it is difficult to deform crystals at low temperatures, $\sigma_p$ is deduced by an appropriate extrapolation to $T=0K$ of the c.r.s.s. The $\sigma_p$ for $\langle 001\rangle \{110\}$ slip in ionic crystals of NaCl-type[6,7] and those for $\{110\} \{110\}$ slip in ionic crystals of NaCl-type[6,7] and those for zinc blende structure (CdTe, HgSe, CuCl, and CuBr[8]) 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, $\langle 110\rangle \{001\}$ slip)[11,12] and Pbs ($\langle 001\rangle \{110\}$ 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 $T=0K$ gives only an upper limit of $\sigma_p$. A crude estimate of $\sigma_p$ for basal slip in $\alpha$-Al2O3 is possible from the data of c.r.s.s. at $T=0K$.[13] The plasticity data of $\alpha$-quartz under hydrostatic pressure at 300-1000°C[14] indicate that $\sigma_p$ of $\alpha$-quartz should be several GPa. For $\alpha$-Al2O3 and $\alpha$-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 data are close to the line A, but the others are far below it. When the c.r.s.s. at $T=0K$ gives only an upper limit of $\sigma_p$. A crude estimate of $\sigma_p$ for basal slip in $\alpha$-Al2O3 is possible from the data of c.r.s.s. at $T=0K$.[13] The plasticity data of $\alpha$-quartz under hydrostatic pressure at 300-1000°C[14] indicate that $\sigma_p$ of $\alpha$-quartz should be several GPa. For $\alpha$-Al2O3 and $\alpha$-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 data are close to the line A, but the others are far below it. When the c.r.s.s. at $T=0K$ gives only an upper limit of $\sigma_p$. A crude estimate of $\sigma_p$ for basal slip in $\alpha$-Al2O3 is possible from the data of c.r.s.s. at $T=0K$.[13] The plasticity data of $\alpha$-quartz under hydrostatic pressure at 300-1000°C[14] indicate that $\sigma_p$ of $\alpha$-quartz should be several GPa. For $\alpha$-Al2O3 and $\alpha$-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 data are close to the line A, but the others are far below it. When the c.r.s.s. at $T=0K$ gives only an upper limit of $\sigma_p$. A crude estimate of $\sigma_p$ for basal slip in $\alpha$-Al2O3 is possible from the data of c.r.s.s. at $T=0K$.[13] The plasticity data of $\alpha$-quartz under hydrostatic pressure at 300-1000°C[14] indicate that $\sigma_p$ of $\alpha$-quartz should be several GPa. For $\alpha$-Al2O3 and $\alpha$-quartz, $h/b$ is assumed to be the widest spacing of atomic planes normal to c-axis.

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