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Correlation of Peierls-Nabarro Stress with Crystal Structure

Takayoshi SUZUKI and Shin TAKEUCHI\*

Institute of Industrial Science and Institute for Solid State Physics\*  
University of Tokyo, Roppongi, Minato-ku, Tokyo 106, Japan

According to the theory of Peierls and Nabarro[1], the Peierls-Nabarro stress  $\tau_p$  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  $\nu$  the Poisson's ratio.

In Fig. 1. are shown the experimental values of  $\tau_p/G$  against  $h/b$ . The  $\tau_p$  of b.c.c. metals (K[2], Fe, Nb, Ta[3], Mo[4]) and a B2 compound  $\beta$ -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  $\beta$ -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,  $\tau_p$  is deduced by an appropriate extrapolation to  $0K$  of the c.r.s.s. The  $\tau_p$  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.<sup>3</sup>He [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  $\tau_p$ . A crude estimate of  $\tau_p$  for basal slip in  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> is possible from the data of c.r.s.s. at 1200-1500°C [13]. The plasticity data of  $\alpha$ -quartz under hydrostatic pressure at 300-1000°C [14] indicate that  $\tau_p$  of  $\alpha$ -quartz should be several GPa. For  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> 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  $\tau_p/G$  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  $\beta$ -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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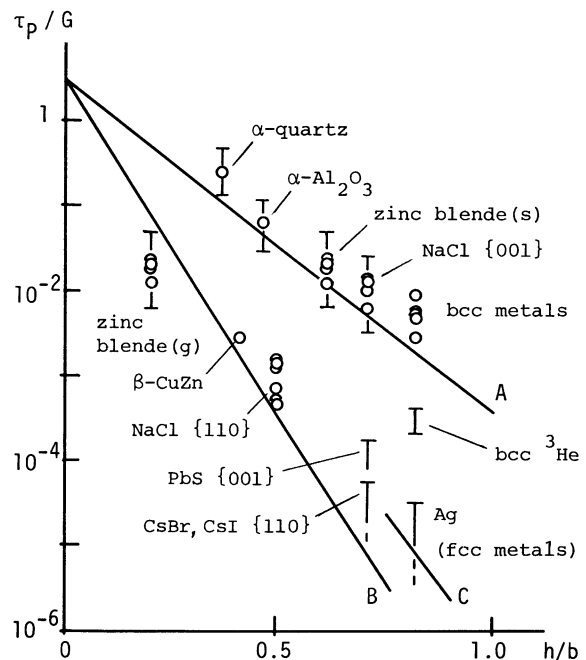


Fig. 1.  $\tau_p$  vs  $h/b$ . Solid lines indicate the relations of eq.(1) for  $\nu=0.3$ . A: for perfect dislocations with Burgers vector  $b$ ; B: for half dislocations with  $b^*=b/2$ , and C: for Shockley partials in f.c.c. lattice with  $b^*=b/\sqrt{3}$ . (s) and (g) for zinc blende structure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