

compared with the observations of Fahlenbrach and co-workers. It is concluded that the observed anisotropy can be rationalized in terms of the slip-induced directional order theory.

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APPENDIX

1. CALCULATION OF BB-PAIRS RESULTING FROM $\{110\}$ $\langle 111 \rangle$ SLIP IN A B2 STRUCTURE

(a) Long-range order — nearest-neighbor case

The long-range ordered B2 structure, Fig. 1(a), consists of two simple cubic sublattices α and β . The total number of BB nearest-neighbor atom pairs in any direction is given by

$$N_{\text{BB}} = N_{\alpha\beta} P_{\text{BB}}(\alpha\beta) + N_{\alpha\alpha} P_{\text{BB}}(\alpha\alpha) + N_{\beta\beta} P_{\text{BB}}(\beta\beta), \quad (\text{A1})$$

where $N_{\alpha\beta}$, $N_{\alpha\alpha}$, and $N_{\beta\beta}$ are the number of bonds joining α and β , α and α , and β with β sites, respectively; and $P_{\text{BB}}(\alpha\beta)$, $P_{\text{BB}}(\alpha\alpha)$ and $P_{\text{BB}}(\beta\beta)$ are respectively the probabilities of a BB pair associated with $\alpha\beta$, $\alpha\alpha$, and $\beta\beta$ bonds.

From the definition of the Bragg and Williams LRO parameter s^{24}

$$s = \frac{r_\alpha - x_A}{1 - x_A} = \frac{r_\beta - x_B}{1 - x_B}, \quad (\text{A2})$$

where

r_α = fraction of α sites (rightly) occupied by A atoms

r_β = fraction of β sites (rightly) occupied by B atoms

x_A = fraction of A atoms in the lattice

x_B = fraction of B atoms in the lattice,

and the definitions

$w_\alpha = 1 - r_\alpha$ = fraction of α sites (wrongly) occupied by B atoms,

$w_\beta = 1 - r_\beta$ = fraction of β sites (wrongly) occupied by A atoms,

we have²⁵, for $x_A = x_B = \frac{1}{2}$,

$$\begin{aligned} P_{\text{BB}}(\alpha\alpha) &= w_\alpha^2 = \frac{1}{4}(1-s)^2 \\ P_{\text{BB}}(\beta\beta) &= r_\beta^2 = \frac{1}{4}(1+s)^2 \\ P_{\text{BB}}(\alpha\beta) &= w_\alpha r_\beta = \frac{1}{4}(1-s^2). \end{aligned} \quad (\text{A3})$$

In the undeformed condition, the distribution of bonds in any of the four nearest-neighbor $\langle 111 \rangle$ directions of the two cells of Fig. 1(a), consists of $N_{\alpha\beta} = 4$, $N_{\alpha\alpha} = N_{\beta\beta} = 0$. Hence $N_{\text{BB}} = 4P_{\text{BB}}(\alpha\beta)$ as calculated from eqn. (A1).

Consider now that a one-step slip has occurred on successive (110) planes in the $[\bar{1}11]$ direction, the configuration of Fig. 1(b) is obtained. In $[\bar{1}11]$ and $[1\bar{1}1]$, which lie on the slip plane, there is no change in pair distribution. Along $[\bar{1}\bar{1}1]$ or $[111]$, which connects the slip planes, the distribution is changed to $N_{\alpha\alpha} = N_{\beta\beta} = 2$, $N_{\alpha\beta} = 0$. Thus the number of BB pairs becomes $N_{\text{BB}} = 2P_{\text{BB}}(\alpha\alpha) + 2P_{\text{BB}}(\beta\beta)$. The increase in BB pairs in $[\bar{1}\bar{1}1]$ or $[111]$ as a result of slip is then

$$\begin{aligned} \Delta N_{\text{BB}} &= 2P_{\text{BB}}(\alpha\alpha) + 2P_{\text{BB}}(\beta\beta) - 4P_{\text{BB}}(\alpha\beta) \\ &= 2s^2 \end{aligned} \quad (\text{A4})$$

upon application of eqns. (A3). Per unit (110) area, we have $\Delta N_{\text{BB}} = s^2/a^2 \sqrt{2}$. A similar expression has been derived previously by Brown and Herman²⁶.

(b) Short-range order — nearest-neighbor case

In the short-range ordered lattice, the nearest-neighbor bonds are no longer identified by α and β sites. In this case, the number of BB pairs is given by

$$N_{\text{BB}} = n \langle P_{\text{BB}} \rangle \quad (\text{A5})$$

where n is the number of bonds and $\langle P_{\text{BB}} \rangle$ is the average probability of a bond being a BB pair. The value of $\langle P_{\text{BB}} \rangle$ is obtained from the Bethe SRO parameter σ^{25} :

$$\sigma = \frac{\langle P_{\text{AB}} \rangle - 2x_A x_B}{\langle P_{\text{AB,max}} \rangle - 2x_A x_B}, \quad (\text{A6})$$

where $\langle P_{\text{AB}} \rangle$ is the average probability of a bond being AB, and $\langle P_{\text{AB,max}} \rangle$ is the value of $\langle P_{\text{AB}} \rangle$ at maximum order. For $x_A = x_B = \frac{1}{2}$, $\langle P_{\text{AB,max}} \rangle = 1$ and thus

$$\sigma = 2(\langle P_{\text{AB}} \rangle - \frac{1}{2}) \quad (\text{A7})$$

The quantities $\langle P_{\text{AB}} \rangle$ and $\langle P_{\text{BB}} \rangle$ are related by the equation¹⁷

$$x_B = \langle P_{\text{BB}} \rangle + \frac{1}{2} \langle P_{\text{AB}} \rangle. \quad (\text{A8})$$

Hence

$$\langle P_{\text{BB}} \rangle = \frac{1}{4}(1 - \sigma). \quad (\text{A9})$$

In the two unit cells of Fig. 1(a), there are $4\langle P_{\text{AB}} \rangle = 1 - \sigma$ BB pairs in any of the four $\langle 111 \rangle$ directions.

After (110)[$\bar{1}\bar{1}1$] slip, Fig. 1(b), the distribution in [$\bar{1}\bar{1}1$] and [$1\bar{1}\bar{1}$] remains unchanged. In [$\bar{1}\bar{1}1$] or [111], $\sigma=0$. Hence the number of BB pairs induced by slip is $\Delta N_{BB}=\sigma$, or $\sigma/2a^2\sqrt{2}$ per unit (110) area, in the [$\bar{1}\bar{1}1$] or [111] direction.

(c) Long-range order — next-nearest-neighbor case

There are three $\langle 100 \rangle$ next-nearest-neighbor directions. One of these, [001], lies on the slip plane, (110), and is not disturbed by slip. The other two, [010] and [100], will alter the atom pair distribution after slip.

In the two unit cells of Fig. 1(a), we have $N_{\alpha\alpha}=N_{\beta\beta}=2$, $N_{\alpha\beta}=0$ before slip, where $N_{\alpha\alpha}$ etc. are now referred to next-nearest-neighbor bonds. After slip, Fig. 1(b), $N_{\alpha\alpha}=N_{\beta\beta}=0$, $N_{\alpha\beta}=4$ in [010] or [100]. Hence the gain in BB pairs in either of these two directions is

$$\Delta N_{BB} = 4P_{BB}(\alpha\beta) - 2P_{BB}(\alpha\alpha) - 2P_{BB}(\beta\beta) = -2s^2, \quad (\text{A10})$$

or $-s^2/a^2\sqrt{2}$ per unit (110) area.

(d) Short-range order — next-nearest-neighbor case

For the next-nearest-neighbor case, the value of $\langle P_{AB,\max} \rangle$ in eqn. (A6) is zero, as complete order results in like-atom pairs in all NNN bonds. We then have, from eqn. (A6),

$$\sigma_2 = 1 - 2\langle P_{AB} \rangle, \quad (\text{A11})$$

with σ_2 denoting the SRO parameter for the NNN case. With the aid of eqn. (A8), eqn. (A11) becomes

$$\langle P_{BB} \rangle = \frac{1}{4}(1 + \sigma_2). \quad (\text{A12})$$

Thus, from Fig. 1(a), the number of BB pairs in [010] or [100] is $4\langle P_{BB} \rangle = 1 + \sigma_2$. After slip, $\sigma_2=0$. Hence the number of BB pairs gained by slip is $\Delta N_{BB} = -\sigma_2$, or $-\sigma_2/2a^2\sqrt{2}$ per unit (110) area.

2. CALCULATION OF BB-PAIRS RESULTING FROM $\{112\}$ $\langle 111 \rangle$ SLIP IN A B2 STRUCTURE

(a) Long-range order — nearest-neighbor case

In the undeformed condition, there are two $\alpha\beta$ bonds per unit cell in each of four $\langle 111 \rangle$ NN directions. After slip, these bonds change to an $\alpha\alpha$

bond and a $\beta\beta$ bond in the three $\langle 111 \rangle$ directions other than the slip direction. Hence $\Delta N_{BB} = P_{BB}(\alpha\alpha) + P_{BB}(\beta\beta) - 2P_{BB}(\alpha\beta)$. When values of eqns. (A3) are entered, we obtain $\Delta N_{BB} = s^2$, or $s^2/a^2\sqrt{6}$ per unit $\{112\}$ area.

(b) Short-range order — nearest-neighbor case

Here, in the undeformed state, the two bonds per cell in each $\langle 111 \rangle$ direction contribute $2\langle P_{BB} \rangle$ pairs of BB bonds. From eqn. (A9), $\langle P_{BB} \rangle = (1 - \sigma)/4$. After slip, $\sigma=0$ and the gain in BB bonds is $\Delta N_{BB} = \sigma/2$, or $\sigma/2a^2\sqrt{6}$ per unit $\{112\}$ area, in the three $\langle 111 \rangle$ directions other than the slip direction.

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