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An analytical expression for the characteristic length scale for randomly faulted hexagonal close-packed structures

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An analytical expression for the characteristic length scale (L) of the pair correlation functions for randomly faulted hexagonal close-packed structures is derived for the case when the roots of the characteristic equation are all real. The values of L obtained by this analytical treatment are in good agreement with those obtained numerically.

Stacking faults are commonly observed in hexagonal and cubic close-packed metals and alloys. They are also observed in several polytypic materials like SiC, ZnS, CdI_2, PbI_2 *etc.* where the positions of one type of atom correspond to the close-packed sphere packing while the other atoms occupy the void sites (Pandey & Krishna, 1992). These stacking faults give rise to characteristic diffuse streaks on diffraction patterns along the $[001]^*$ direction for those $HK.L$ reciprocal-lattice rows for which $H - K \neq 0 \bmod 3$ (Wilson, 1962). The effect of stacking faults on diffraction patterns can be modelled through various analytical (Wilson, 1962; Warren, 1969; Pandey & Krishna, 1992) and Monte Carlo methods (Berliner & Werner, 1986; Kabra & Pandey, 1995, 1996; Shreshtha *et al.*, 1996). In all these approaches for calculating diffraction effects due to stacking faults, the pair correlation functions are first obtained, whose Fourier transforms give the diffracted intensity. Through the use of kinetic Ising models for modelling restacking transitions between close-packed structures, Shreshtha & Pandey (1996, 1997) and Shreshtha *et al.* (1996) showed that the pair correlation functions $P(m)$, $Q(m)$ and $R(m)$ (which describe the probabilities of occurrence of A–A, B–B, C–C; A–B, B–C, C–A; and A–C, B–A, C–B pairs of layers separated by m layers) for faulted close-packed structures can be described by exponentially varying functions like $\exp(-m/L)$, where L is a characteristic length scale. By scaling the interlayer separation with respect to this characteristic length scale, the various pair correlation functions in the time domain were shown to collapse into master curves (Shreshtha *et al.*, 1996). Recently, we demonstrated that the scaling behaviour holds true in the fault probability domain as well (Tiwary & Pandey, 2007), where this was shown for random distributions of growth and deformation faults and their mixtures in hexagonal close-packed (h.c.p.) crystals. The characteristic length scales were obtained through Monte Carlo simulations as well as through numerical and analytical procedures by considering the characteristic equation for random faults in h.c.p. crystals (Pandey & Krishna, 1977). It is known that the roots of the characteristic equation can be real or complex depending on the values of the fault probabilities (Pandey & Krishna, 1977). We obtained analytical solutions for the case where the roots are complex but we were unable to do so for the case when the roots were real, for which we had to resort to numerical procedures (Tiwary & Pandey, 2007). In this communication, we demonstrate that it is possible to obtain an analytical solution for this case (real roots) as well, and calculate the dependence of characteristic length scale on fault probabilities through this analytical route.

The characteristic equation for h.c.p. crystals with random growth fault probability α and random deformation fault probability β is given as (Pandey & Krishna, 1977)

$$\rho^2 + \alpha\rho - (1 - 2\alpha)(1 - 3\beta + 3\beta^2) = 0. \tag{1}$$

We assume that the solutions ρ_1 and ρ_2 for equation (1) are given by $\rho_1 = Z\exp(i\theta)$ and $\rho_2 = Z\exp(-i\theta)$, where Z and θ are

$$Z = \frac{\alpha^2 - x^2}{4} \tag{2}$$

$$\theta = \arctan\left(\frac{4Z^2 - \alpha^2}{-\alpha}\right)^{1/2}, \tag{3}$$

where

$$x = \left(\{\alpha - 4(1-\gamma) - 2[(3-4\gamma)(1-\gamma)]^{1/2}\} \times \{\alpha - 4(1-\gamma) + 2[(3-4\gamma)(1-\gamma)]^{1/2}\}\right)^{1/2} \tag{4}$$

and

$$\gamma = 3\beta(1-\beta). \tag{5}$$

The pair correlation function $P(m)$ will thus be (Pandey & Krishna, 1977)

$$P(m) = 1/3 + (2/3)\{C_e\rho_e^m + C_o\rho_o^m\}, \tag{6}$$

where

$$C_e = \tfrac{1}{2}\left(1 + \frac{1-\alpha}{x}\right), \tag{7}$$

$$C_o = \tfrac{1}{2}\left(1 - \frac{1-\alpha}{x}\right). \tag{8}$$

Let us consider the specific case of pure random growth faulting first, with $\alpha < 0.536$, which was considered analytically intractable by Tiwary & Pandey (2007). In this region, the pair correlations are known to be purely h.c.p. type, and thus we focus only on the even values of m, which yield purely decaying type pair correlation functions. For even m, it can easily be shown that

$$P(m) = 1/3 + (2/3)\left(\frac{\alpha^2 - x^2}{4}\right)^{m/2}\left\{C_e\left(\frac{(\alpha - x)^2}{\alpha^2 - x^2}\right)^{m/2} + C_o\left(\frac{(\alpha + x)^2}{\alpha^2 - x^2}\right)^{m/2}\right\}. \quad (9)$$

For $0 < \alpha < 0.536$, we have

$$\frac{(\alpha - x)^2}{\alpha^2 - x^2} \ll 1 \ll \frac{(\alpha + x)^2}{\alpha^2 - x^2}. \quad (10)$$

Thus, the first term inside the braces in equation (9) is negligible compared to the second term, and hence

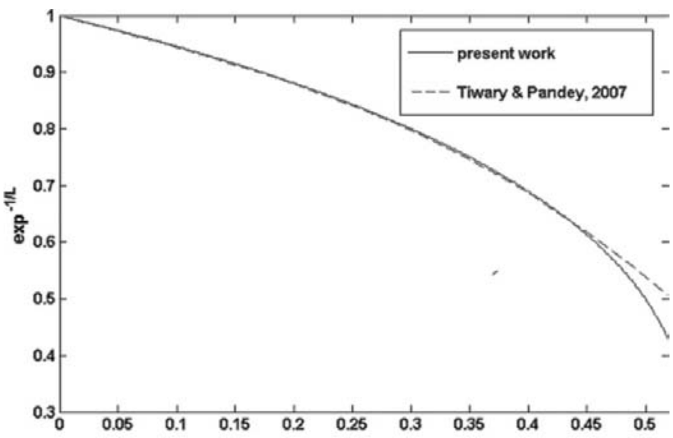

Figure 1
Variation of $\exp(-1/L)$ with the growth fault probability α for pure random growth faulting with $0 < \alpha < 0.536$.

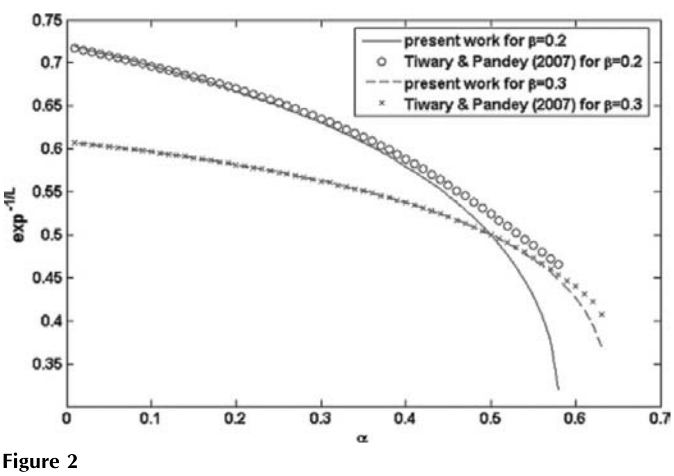

Figure 2
Variation of $\exp(-1/L)$ with the growth fault probability α for mixed faulting, with deformation fault probability $\beta = 0.2$ and $\beta = 0.3$.

$$P(m) \approx 1/3 + (2/3)\left(\frac{\alpha^2 - x^2}{4}\right)^{m/2}\left\{C_o\left(\frac{(\alpha + x)^2}{\alpha^2 - x^2}\right)^{m/2}\right\} \quad (11)$$

or

$$P(m) = 1/3 + (2/3)C_o\left(\frac{\alpha + x}{2}\right)^m. \quad (12)$$

Using the following exponential functions to describe the dependence of $P(m)$ on m (Shreshtha & Pandey, 1996),

$$P(m) = 1/3 + (2/3)\exp(-m/L), \quad \text{for } m \text{ even}, \quad (13)$$

and

$$P(m) = 1/3 - (1/3)\exp(-m/L), \quad \text{for } m \text{ odd}, \quad (14)$$

and, by comparing equation (13) with equation (12), we obtain the desired analytical expression for the characteristic length scale:

$$L = \frac{-1}{\log[(\alpha + x)/2]}. \quad (15)$$

The functional dependence of L on α as obtained through equation (13) for the case of pure random growth faulting with $\alpha < 0.536$ is shown in Fig. 1. Fig. 1 also shows the dependence of L on α for $\alpha < 0.536$ as obtained by Tiwary & Pandey (2007) through exact numerical calculations. It is evident from this figure that the two curves are in excellent agreement up to about $\alpha = 0.45$. The small departure for $\alpha > 0.45$ shows that the approximation given by equation (10) is not adequate. Although we have considered the case of pure growth faults in this communication, our results are valid for the entire region A of Fig. 1 of Tiwary & Pandey (2007) even when there are coexisting deformation faults as well. Fig. 2 compares the cases of mixed fault probabilities with $\beta = 0.2$ and 0.3. Once again, the analytical results are in excellent agreement with the numerically computed values for $\alpha < 0.4$.

References

Berliner, R. & Werner, S. A. (1986). *Phys. Rev. B*, **34**, 3586–3603.
Kabra, V. K. & Pandey, D. (1995). *Acta Cryst.* A**51**, 329–335.
Kabra, V. K. & Pandey, D. (1996). *Phase Transit.* **59**, 199–206.
Pandey, D. & Krishna, P. (1977). *J. Phys. D*, **10**, 2957–2968.
Pandey, D. & Krishna, P. (1992). *International Tables for Crystallography*, Vol. C, edited by A. J. C. Wilson, pp. 660–667. Dordrecht: Kluwer.
Shreshtha, S. P. & Pandey, D. (1996). *Europhys. Lett.* **34**, 269–274.
Shreshtha, S. P. & Pandey, D. (1997). *Proc. R. Soc. London Ser. A*, **453**, 1311–1330.
Shreshtha, S. P., Tripathi, V., Kabra, V. K. & Pandey, D. (1996). *Acta Mater.* **44**, 4937–4947.
Tiwary, P. & Pandey, D. (2007). *Acta Cryst.* A**63**, 289–296.
Warren, B. E. (1969). *X-ray Diffraction.* New York: Addison Wesley.
Wilson, A. J. C. (1962). *X-ray Optics.* New York: John Wiley.