For cuprite, the literature (Tromans & Meech, 2001) suggests that the main slip system is ⟨001⟩{100}. The contrast factor can be calculated analytically from the single-crystal elastic constants of cuprite (c_{11} = 121, c_{12} = 105 and c_{44} = 12.1 GPa; Every & McCurdy, 1992*b*) following Martinez-Garcia *et al.* (2007):

$$\overline{C}_{\mathrm{Cu_2O},e} = 0.355963 - 0.609491\,\frac{h^2k^2 + k^2l^2 + h^2l^2}{(h^2 + k^2 + l^2)^2}, \qquad (3.6.58)$$

$$\overline{C}_{\mathrm{Cu_2O},s} = \frac{2}{3}\frac{h^2k^2 + k^2l^2 + h^2l^2}{(h^2 + k^2 + l^2)^2}. \qquad (3.6.59)$$

For tenorite, a different approach was followed. The phase is minor and the single-crystal elastic constants are not readily available: we can therefore use the contrast factor in an effective way by refining the coefficients of the corresponding invariant [see equation (3.6.42)]. This preserves the profile shape determined by Wilkens' theory and just dilutes the meaning of the dislocation density. The average contrast factor is

$$\begin{aligned}\overline{C}_{\mathrm{CuO},\{hkl\}} &= \Big\{4\big[E_1h^4 + E_2k^4 + E_3l^4 + 2(E_4h^2k^2 + E_5k^2l^2 + E_6h^2l^2) \\ &\quad + 4(E_7h^3k + E_8h^3l + E_9k^3h)\big]Y^4Z^4\sin^4\beta\Big\} \\ &\quad \times \left(\left\{k^2Z^2 + 2Y^2(l^2 + h^2Z^2) - Z[4hlY^2\cos(\beta) + k^2Z\cos(2\beta)]\right\}^2\right)^{-1}, \end{aligned} \qquad (3.6.60)$$

where a, b, c and β are the unit-cell parameters of tenorite, $Y = b/a$ and $Z = c/a$.

The dislocation density in Cu_2O is quite high [ρ = 2.8 (5) × 10^{16} m^{-2}]: dislocations are more of the edge character [f_E = 0.85 (3)] and the outer cutoff radius R_e = 9 (3) nm leads to a Wilkens' parameter of approximately 1.5, suggesting a strong dislocation interaction. The high dislocation density in this material is justified by the very low shear modulus (G = 10.3 GPa; Every & McCurdy, 1992*b*), whereas the high dislocation interaction is the result of the severe deformation induced by the milling.

APPENDIX A3.6.1
Functions for profile shapes

The unit-area Gaussian $G(x, \omega)$ and Lorentzian $L(x, \omega)$ functions are defined as

$$G(x, \omega) = \frac{2\sqrt{\ln 2/\pi}}{\omega}\exp\left(-\frac{4x^2\ln 2}{\omega^2}\right), \qquad (3.6.61)$$

$$L(x, \omega) = \frac{2}{\pi\omega}\left(\frac{1}{1 + 4x^2/\omega^2}\right), \qquad (3.6.62)$$

where x is the running variable and ω is the full-width at half-maximum. Based on these definitions, the Voigt and pseudo-Voigt are

$$V(x, \omega_L, \omega_G) = L(x, \omega_L) \otimes G(x, \omega_G) \qquad (3.6.63)$$

and

$$\mathrm{pV}(x, \omega_L, \omega_G) = \eta L(x, \omega_L) + (1 - \eta)G(x, \omega_G), \qquad (3.6.64)$$

respectively, where η is the mixing parameter (ranging between 0 and 1) and w_L and w_G are the width of the Lorentzian and Gaussian components, respectively.

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