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Response to Zbigniew Kaszkur's comment on the article *The nanodiffraction problem*

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In a previous article (Öztürk *et al.*, 2015) we showed that the classical Lorenz factor ($L_F = 1/\cos\theta$) and its extensions are inapplicable for correcting diffraction patterns from nanoparticles with diameters, D, smaller than 20 nm. However, Kaszkur (2019) suggests that in our article *The nanodiffraction problem* (Xiong *et al.*, 2018) 'the correct comparison should be made between the thin-film case and the Debye formula multiplied by $\sin(2\theta)$'. This factor, termed the 'single-crystal Lorenz factor', accounts for the change in the irradiated volume of the crystal as a function of 2θ (Reynolds, 1986). Since the diffraction patterns in our previous article were simulated assuming an infinite number of crystallites in the powder diffraction analysis, and an infinitely large slab of finite thickness irradiated by a plane wave for the thin-film case, we do not consider such a correction theoretically justified. Nevertheless, we tested Kaszkur's hypothesis using numerical simulations. Fig. 1(*a*) shows the expected diffraction pattern for a monodisperse powder sample consisting of infinitely many, ideal, Au spheroids, 5 nm in diameter, computed using the modified Debye formalism (https://github.com/wojdyr/debyer) with Cr $K\alpha$ radiation. The variation of the suggested correction factor, $C_F = \sin(2\theta)$, over this angular range and the corrected intensity profile obtained by multiplying the Debye intensity profile with this factor are also plotted. In Fig. 1(*b*) the lattice parameter errors, $\Delta a_{hkl} = a_{hkl} - a_{ideal}$, computed from the individual peak positions for these two profiles are shown. We do not see any improvement over the uncorrected results. We observed similar results for (corrected) patterns computed using other wavelengths and for full-pattern fitting. For larger-diameter ($D > 20$ nm) particles, we recovered the original lattice parameter without using any corrections. We conclude that (i) applying the 'Lorenz correction' to computed nanoparticle powder patterns requires further study and (ii) the hypothesis put forward by Kaszkur (2019) cannot be used to correct the patterns reported in our current article (Xiong *et al.*, 2018). We hope that our

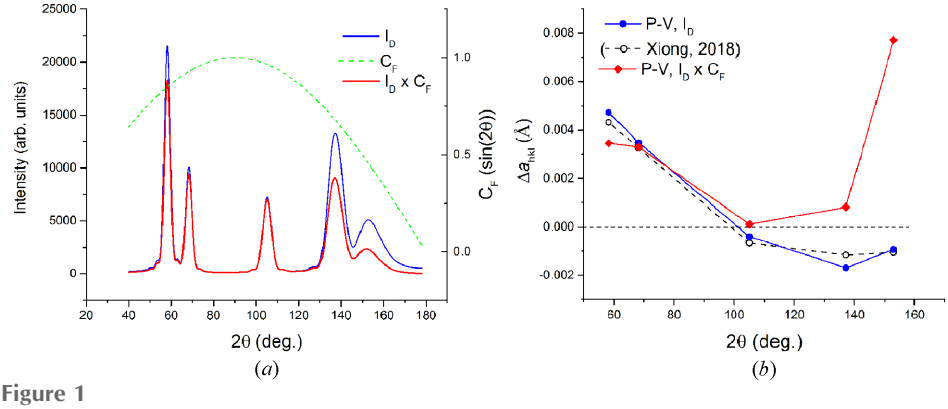

Figure 1
(*a*) Diffraction patterns for 5 nm-diameter ideal Au spheroids, computed using the Debye formalism with Cr $K\alpha$ radiation and after correction. The variation of the correction factor, $C_F = \sin(2\theta)$, over this angular range is also plotted. (*b*) The deviation of the unit-cell parameters, Δa_{hkl}, from the ideal Au lattice parameter used in the simulation. Identical procedures utilizing pseudo-Voigt functions over identical ranges and background functions were used to fit both profiles. Δa_{hkl} values reported in our original article are also included for reference (Xiong *et al.*, 2018), since a different version of the fitting program, no longer available to us, was used at the time.

article, and this exchange in *Journal of Applied Crystallography*, will stimulate the development of a rigorous theoretical framework for the analysis of nanocrystalline diffraction patterns. Until such a framework is in place, diffraction analysis results from such systems should be treated with caution given, also, that significant details of the distribution of unit-cell parameters within nanoparticles are eliminated during diffraction averaging (Xiong *et al.*, 2019).

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