Phonon Scattering in High-Resolution Electron Microscopy

C.B. Boothroyd

IMRE, 3 Research Link, Singapore 117602

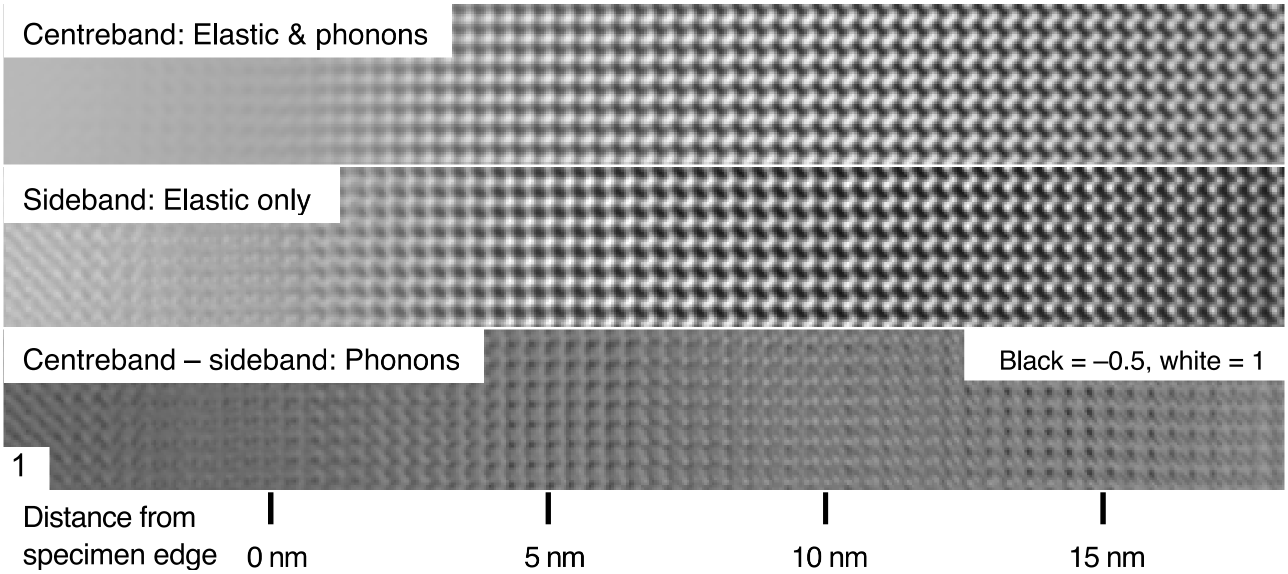
It is generally accepted that the lattice fringe contrast in experimental high-resolution electron microscope (HREM) images is lower than that in image simulations by a factor of between 2 and 6 [1]. One likely reason for this discrepancy is the contribution phonon, or thermal diffuse, scattering makes to lattice images. Electrons scattered by phonons are visible as diffuse scattering between the Bragg spots in the diffraction pattern and the loss in intensity of the Bragg spots is modeled by the Debye-Waller factor in image simulations. However, the additive effect of this diffuse scattering on images is not taken into account by image simulations. The amount of phonon scattering as a function of specimen thickness has been measured both for Si by convergent beam diffraction [2] and for ZrB_{12} by electron holography [3] and in both cases found to contribute about 10% of the total intensity at a thickness typically used in high resolution imaging.

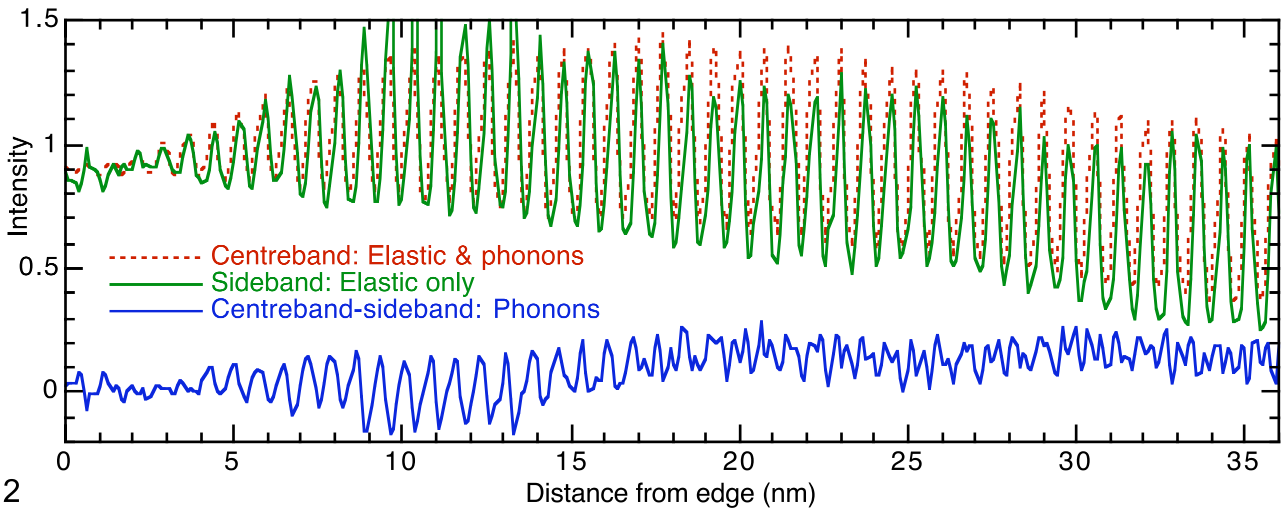
In this paper the effect of the contribution of phonon scattering on the pattern of lattice images in ZrB_{12} is investigated using electron holography. The energy loss associated with phonon scattering is ~0.025 eV and is too small to be excluded by energy filters. In electron holography the lattice image is interfered with a reference wave which has passed around the specimen. Constructive interference fringes (the sideband), can only arise when there is no energy loss within the specimen, so the amplitude of the hologram fringes provides a measure of elastic scattering (fig. 1 middle). A normal lattice image can be obtained by using Fourier filtering to remove the hologram fringes then subtracting the reference wave intensity. The resulting image (the centreband, fig. 1 top) is identical to a normal lattice image and, provided the original hologram was energy filtered to remove plasmon and higher losses, contains both elastic and phonon scattering. The contribution of phonon-scattered electrons (fig. 1 bottom) can be obtained by subtracting the sideband (elastic only, fig. 1 middle) from the centreband (elastic plus phonons, fig. 1 top).

It can be seen from fig. 1 that the centreband and sideband lattice images are very similar to each other, with the most obvious difference being a significant increase in contrast for the sideband image. This is consistent with the phonon scattering contribution being only about 10% of the total and can be seen more clearly in the linescans in fig. 2. Fig. 3 shows single unit cells cut from images similar to fig. 1 for a range of defoci and confirms that lattice images including phonon scattering (fig. 3a) have less contrast but similar patterns to those excluding phonon scattering (fig. 3b). More interesting are the phonon scattering images (fig. 3c) which all show lattice fringe contrast. For all defoci the phonon lattice images are of opposite contrast to the elastic images, ie bright where the elastic images are dark. Thus phonon scattering has reversed contrast and so reduces the lattice fringe contrast by *more* than the usual assumption of a constant background would suggest.

References

[1] C.B. Boothroyd, *J. Microsc*. 190 (1998) 99.
[2] C.B. Boothroyd and M. Yeadon, *Ultramicroscopy* 96 (2003) 361.
[3] C.B. Boothroyd and R.E. Dunin-Borkowski, *Ultramicroscopy* 98 (2004) 115.
[4] Many useful discussions with Rafal Dunin-Borkowski are gratefully acknowledged.





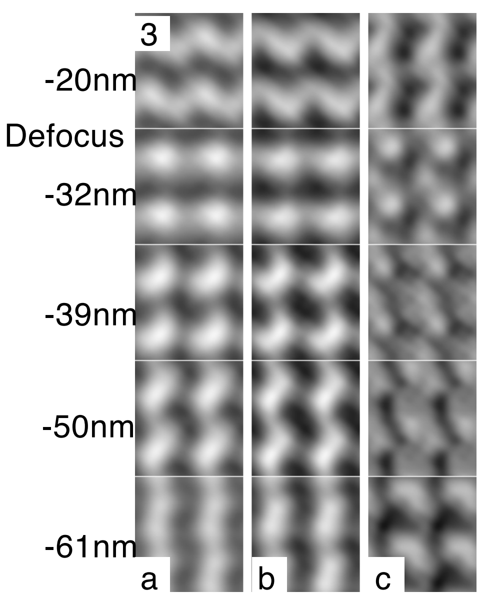


FIG. 1. Lattice images of ZrB_{12} (cubic, a = 0.74 nm) for defocus –39nm. The raw sideband image is particularly noisy, so these images were lattice averaged over blocks of 7 by 21 unit cells. Black = 0, white = 1.5, except for phonon image.

FIG. 2. Linescans through peaks in lattice images shown in fig 1 for defocus –39nm.

FIG. 3. Experimental lattice averaged images of single ZrB_{12} unit cells for defoci from –20 to –61 nm. a, Centreband: elastic & phonons, b, Sideband: Elastic only and c, Centreband–sideband: Phonon scattering only. a and b, black = 0, white = 1.5, c, black = –0.2, white = 0.5