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QCBED Measurements of Vacancy Concentrations, Lattice Contraction, and Bonding Electron Densities Surrounding Aluminium Nanovoids

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Background incl. aims
We set out to make the first position-resolved measurements of bonding electron density around a nanostructure in an inhomogeneous crystalline material.

All bonding electron density and potential studies to date have only involved homogeneous, single phased materials; however, most materials that serve us have hybridised properties because of the nanostructures that they contain, often by design. We also note that materials defects are ubiquitous and unavoidable, so the assumption that we can derive materials properties from notionally perfect regions of single, homogeneous crystal is limited in scope and "real" applications. This work aims to provide a new capability for interrogating bonding electron densities around nanostructures in nanostructured and inhomogeneous materials. Our first attempt involves nanovoids in nominally pure (99.9999+%) aluminium.

On the way to realising this aim, we have made several discoveries as a result of having to accurately map vacancy concentrations and determine the associated lattice contraction due to vacancies in order to be able to measure the Fourier coefficients (structure factors) of the crystal potential and electron density precisely and accurately (to <0.1% uncertainty).

Methods

Over the last 15 years, we have developed a multislice [1,2] approach to quantitative convergent-beam, electron diffraction (QCBED) refinements. We call this method QCBEDMS. This has facilitated the necessary analyses to generate the results summarised below. For more details regarding the method, please come to the talk – they will not be discussed here.

Results

From 45 CBED patterns collected through many different voids and the surrounding matrix, in different orientations and with different electron energies:

- We measured the volume of a vacancy with 5-fold less uncertainty than previous work.
- Observed that nanovoids in aluminium can "heal" even after significant beam damage.
- We mapped vacancy concentrations around aluminium nanovoids in 3 dimensions.
- We have shown that the bonding electron density around aluminium nanovoids is diluted by the elevated vacancy concentration surrounding these voids.

Conclusion

Our work and the results from it are a precursor to measuring and mapping bonding electron densities around many other types of nanostructures (eg. nano-precipitates) in other nanostructured, inhomogeneous materials. Furthermore, we are confident that our technique can be extended to mapping solute atom concentrations around such structures and that this will go together with accurate bonding electron density measurements within and surrounding these features in other nanostructured materials.

Keywords:

QCBED, multislice, bonding electron densities

Reference:

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