Extending Geometric Phase Analysis (GPA) to measure elastic stresses and strains across nanocrystals, grain boundaries and heterostructures

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Geometric phase analysis (GPA) of HR(S)TEM images has become a standard technique for strain mapping over the years [1]. Whilst successful, the approach is not without limitations. An internal reference of undisturbed crystal must be present within the field of view and the regions of crystal to be analysed must have common, or closely related, reciprocal lattice vectors. Here, we present a major extension of GPA that overcomes these problems allowing the study of nanocrystals, where no reference region is generally present, grain boundaries and epitaxial heterostructures. The new theory has the added advantage of correcting errors due to global optical distortions and is general to any stain mapping technique. It is little known, for example, that a global shear applied to an image will disturb conventional strain analysis.

We start from the principle that elastic strain is measured with respect to the relaxed crystal structure. By introducing the notion of crystallography to GPA, we will show how a reference image of known uniform crystal can be used to define the optical distortions and absolute magnification. An experimental image taken under identical conditions can then be analysed to determine the local elastic strain, independently of the in-plane orientation of the crystal. Large rotations across grain boundaries and domain walls will be accommodated by the new procedure. The local stresses can then be determined from elastic theory. We will implement the theory, which has been incorporated in the latest version of GPA from HREM Research Inc., for some representative examples.

[1] M.J. Hÿtch, E. Snoeck and R. Kilaas, Ultramicroscopy 74 (1998) 131 - 146.