Computational tools for the atomic-scale analysis of quasicrystals using atom probe microscopy

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Quasicrystals have rotational order but no translational periodicity. The first documented study of quasicrystals was published in 1984 using transmission electron microscopy [1]. Since their discovery, several diffraction techniques (electron, neutron, x-ray) have been applied to study the atomic-scale structure of quasicrystals [2-4]. These techniques offer averaged information in the reciprocal space of the bulk crystal.

Atom probe microscopy (APM) includes tomographic and other imaging techniques that provide localised information at the atomic scale in real space. With the chemical information and 3D positions of each atom in a ~100 million-atom dataset, access to information about the local atomic neighbourhoods becomes available with statistical certainty. These techniques have not been widely applied to the study of stable quasicrystals. Field ion microscopy images, for example, have been published [5,6], and metastable quasicrystal phases within amorphous systems or steels have also been studied [7]. However, given the significant development of APM techniques over the past two decades [8], and in particular the development of atom probe crystallography [9], this work sought to extract localised atomic-scale structural information from quasicrystals.

Here, a data analysis procedure for an AlMnPd stable quasicrystal is reported. We describe the specimen preparation procedure and the atom probe experimental parameters. We define the mathematical formalisms, and the computational tools required to measure the local atomic structure from atom probe data.

References:

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