Isotopic Substitution Neutron Diffraction for Enhanced Structural Information from Crystalline Powder Materials

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Why bother determining the structure of a material?

The usual answer is that structure is key in determining the properties of the material. Powder diffraction techniques allow rapid assessment of readily available polycrystalline materials. Small differences in structural features, such as the level and distribution of dopants, changes in bond lengths/angles as a function of temperature and thermal displacements of atoms, all influence properties. Therefore, to fully understand a material, extraction of the highest quality structural information is crucial.

Using isotopically substituted samples and combined data-set analysis it is possible to extract structural information of unprecedented quality from polycrystalline materials. Uses of isotopic substitution to overcome absorption effects (*e.g.* ^{7}Li, ^{11}B, ^{154}Sm and ^{160}Gd) and incoherent scattering problems (*e.g.* ^{2}H) are well established, however, using the contrast in the scattering lengths of isotopes of an element to obtain enhanced structural information has been almost exclusively restricted to local structure investigations of non-crystalline materials and liquids. For over half of stable elements there exist, at reasonable cost (between $1 and $5 per mg), two or more isotopes with strongly contrasting scattering lengths.

Several published examples of the usefulness of the technique are presented with a brief introduction.

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