CALCULATION OF ION CHANNELING DIRECTIONS IN LOW SYMMETRY OPTICAL MATERIALS

D. B. POKER

Solid State Division, Oak Ridge National Laboratory*, Oak Ridge, TN 37831-6057.

Rutherford backscattering spectroscopy along ion channeling directions is useful for numerous applications in the characterization of all types of materials, due to its sensitivity to interstitial location, lattice quality, and composition. The determination of channeling directions and sample orientation in materials with high symmetry lattices is usually straightforward. However, many optical materials have relatively low crystal symmetry, which complicates the determination of likely directions for ion channeling. This is especially true of electrooptic materials, such as LiNbO_3 , which lack inversion symmetry. Therefore, an algorithm for the calculation of likely channeling directions in low symmetry lattices has been developed.

The algorithm creates a virtual three-dimensional atomic structure from lattice and basis data input by the user. The sizes of atoms within the lattice can be varied to represent relative ion scattering cross sections. The optical transmission of the structure in the hard sphere approximation is calculated for an array of angular orientations. A stereographic projection of the data can be used to display the relative channeling probabilities of the crystal. The correlation between optical transmission and channeling yield, and the application of the algorithm to planar as well as axial channeling will be discussed.

* Operated by Martin Marietta Energy Systems, Inc. under Contract No. DE-AC05-84OR21400 for the U.S. Department of Energy.