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Solid State NMR, Diffraction and Modeling of Intermetallics

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Intermetallic compounds are a fascinating class of materials with respect to structural chemistry and technological applications. The interest of basic research focuses on chemical bonding and local ordering of the atoms. Combined application of NMR spectroscopy, quantum mechanical calculations of NMR parameters based on density functional theory (DFT), and X-ray diffraction was applied to study the peculiarities of the Ga bonding situation in alkaline earth metal gallides [1,2]. The compounds were chosen as a model system to determine reliable NMR spectroscopic parameters for the investigation of intermetallic compounds possessing metallic conductivity. Very good agreement of calculated and experimental parameters was achieved. An analysis of the electric field gradient (EFG) contributions reveals its local character. It is determined by the population difference of the p-like states of the electrons of the Ga atoms. Due to the reliability of the EFG for the investigation of intermetallic compounds studies of the influence of disorder on the local bonding situation of the Ga atoms in the solid solutions of $Sr_{1-x}Ba_xGa_2$ and were chosen in a next step. Super lattice structures were derived from the crystal structures of the binary parent phases to model the varying local arrangements of the atoms. DFT calculations based on these super lattice models enabled the theoretical deamination of the EFG in a good agreement with the experimental values. Thus, the EFG can also be used to study local arrangements of the atoms in disordered materials possessing metallic conductivity. The anisotropic conductivity of the powder samples can be used to align the crystallites in the magnetic field resulting in an increased experimental resolution. Line shape analysis of orientation dependent NMR experiments of $M(Al_{1-x}Ga_x)_4$ with M = Sr, Ba reveal local ordering of the Al atoms.

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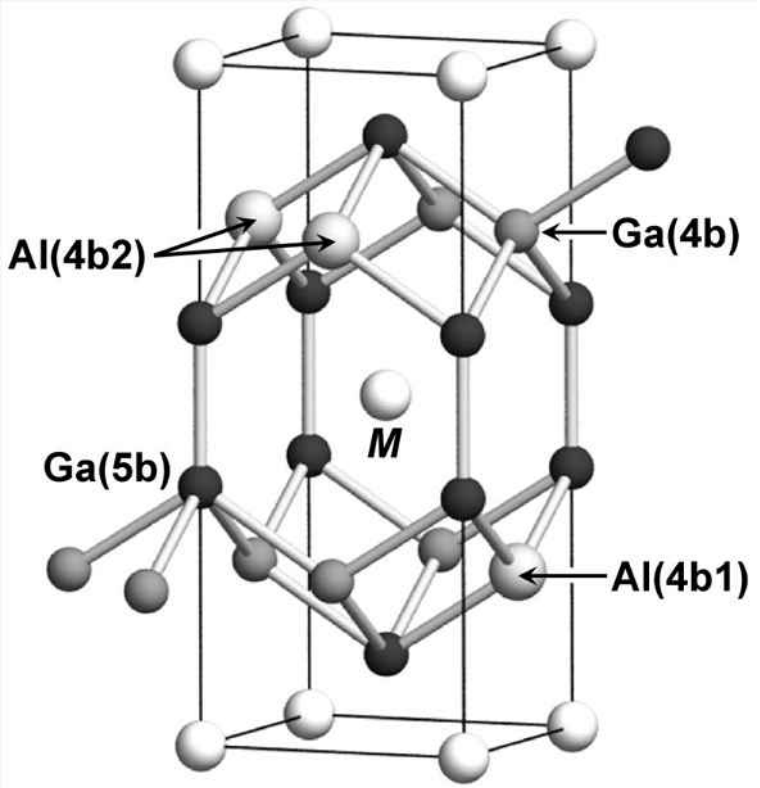

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