
Keywords: electron density, synchrotron radiation, band structure.

CaNi$_2$Si$_2$ crystallises in the ThCr$_2$Si$_2$ type structure, one of the most frequently observed structures in ternary compounds with the formula RT$_2$X$_2$ (R alkaline earth or lanthanide element; T transition metal and X an element from group 13 to 16).

Concerning the silicides only the compounds containing manganese are magnetic, showing a great variety of behaviour ranging from ferromagnetism to antiferro-magnetism and canted magnetic structures.

This study is the first of a series in which we want to analyse the electron density of a several compounds with a good accuracy. In the present report we compare with the results of a Full-Potential-Linearised-APW calculation of the band-structure and the valence electron density distribution.

The X-ray diffraction measurement was carried out at the four-circle diffractometer D3 at HASYLAB using a wavelength of 0.4 Å. This choice was made because of the high absorption of this dense compound and the small size of the sample. The analysis of the experimental data is also complicated by the high symmetry of the structure (I4/mmm) with all atoms in highly symmetric special positions. The consequence is that certain classes of reflections are systematically weak and difficult to measure with a good accuracy.

Although the diffraction data are rather insensitive to diffuse components of the electron density, there is nevertheless a good agreement between theory and experiment.

A weak covalent Si-Si bond interaction is observed, but most pronounced is the preferred occupation of the nickel 3d-orbitals.