Structural modifications of Gd-Au-Si quasicrystal approximants

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Gold-based Tsai-type approximants in the RE-Au-p (p=Si, Ge, Al) systems have lately attracted much attention due to their long-range magnetic order at low temperatures.[1-3] In order to fully model and understand the magnetic interactions in these materials, it is of paramount importance to first have full understanding of their nuclear structures. In this work, we present three previously unknown structural modifications of Tsai-type Gd-Au-Si approximants, and how these structural differences result in different magnetic behavior at low temperatures. The nuclear structures were studied by single crystal X-ray diffraction and neutron diffraction intensities were collected at the D9 beamline at ILL to investigate the magnetic structure of one of these structural modifications. A very short wavelength (0.5 Å) was chosen for the neutron experiment, in order to minimize the strong absorption effects of Gd. The preliminary results indicate a magnetic structure, which differs from that of other RE-Au-Si approximants.

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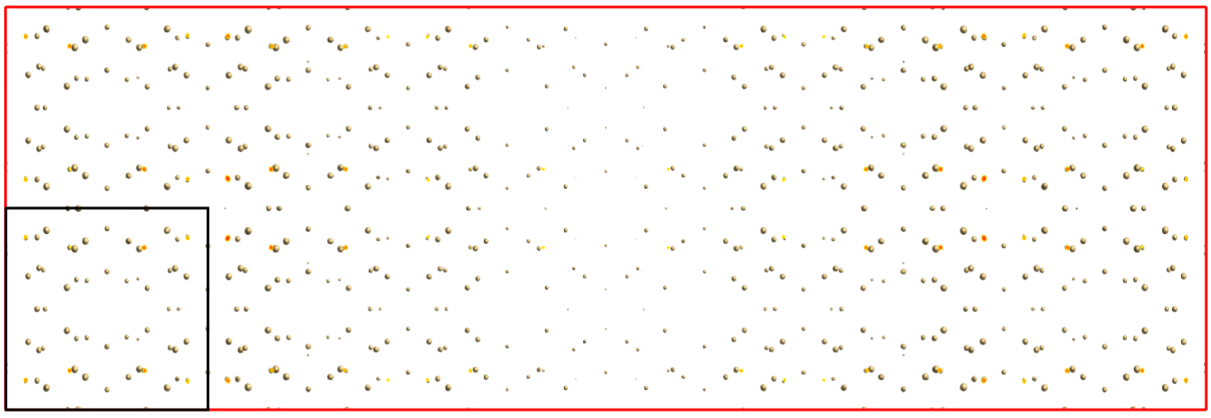

Fig.1: Electron density isosurfaces showing the density variation in the supercell (red) of a Gd-Au-Si approximant along the 88.5 Å period. The basic 14.72 Å cubic unit cell is outlined in black.