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MS22-P2 Charge density and disorder in Al_2Ru

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The simple intermetallic compound $RuAl_2$ exhibits remarkable physical properties, e.g. it is an unconventional semiconductor with narrow bad gap [1]. In terms of structural features it is considered a parent structure and main building block for the family of Nowotny chimney Ladder (NCL) structures [2]. In contrast to the intriguing structures of most NCL compounds, the adopted $TiSi_2$ type structure is 'well behaved' as it is not modulated and therefore composite structure approach needs not to be applied [3]. In order to avoid problems due to inelastic scattering with Ag-target X-ray sources and in order to collect Bragg intensities up to very high resolution, diffraction data were collected at beamline ID-15-B of the Advanced Photon Source applying 30 keV X-rays. Since a large fraction of possible Bragg reflections is systematically weak, special efforts were necessary in order to extract reliable intensities from measured images. The fundamental approach as implemented in EVAL15 finally gave very good results [4]. The independent atom refinement already derives a model with excellent agreement, however, a faint indication of specific disorder is revealed. After applying the multipolar model according to Hansen and Coppens using XD-2006 [5], charge transfer from Al atoms towards Ru is clearly derived. Al_2Ru obviously is a more adequate description in perfect agreement with Si_2Ti as given in the early determination of the parent structure [6]. Details of chemical bonding along with interpretation of detected disorder in terms of stacking faults will be discussed. Similar deviations in typically well-known structures seem to be quite common and deserve careful consideration.

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