Charge density analysis of α-Manganese

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The crystal structure of α-Manganese, the allotropic form stable at ambient conditions, is quite unusual among metals and elements. Due to its complexity with four distinct atomic sites and associated variation in local symmetry and coordination number it may be considered as a prototype for intermetallic compounds. Even more, it is among the very few structures of elements lacking a center of symmetry. However, it seems an attempt to assign the associated absolute structure has never been described. Our results afford quite a surprise in this respect. As inequivalent atomic sites provide for internal scaling and thus for minimizing certain systematic errors, α-Manganese looks like a very interesting candidate for a charge density analysis. First results in our efforts to reconstruct the electron distribution from X-ray diffraction data will be discussed.