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SAED and HREM Studies of Zr_2Co_{11} Intermetallic Compound

X.Z. Li[1], W.Y. Zhang[1,2] and D.J. Sellmyer[1,2]

[1.] Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588
[2.] Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588

Rare-earth-free permanent-magnets have gained immense focus in the view point of mitigating the critical-material aspects of rare-earth elements. The intermetallic compound Zr_2Co_{11} is a promising candidate. Polymorphism exists in the Zr_2Co_{11} compound; a high-temperature phase has a rhombohedral structure and a low temperature phase has an orthorhombic structure [1,2]. Both of the two phases in relative small grain sizes have been observed often in the same rapidly quenched samples. In this case, selected-area electron diffraction (SAED) and high-resolution electron microscopy (HREM) are the suitable experimental techniques to study the crystalline structures. Theoretical calculations predict that the lowest-energy structures near Zr_2Co_{11} composition share a common structural motif [3]. The combination of theoretical and experimental results allows correct structural models of the two Zr_2Co_{11} phases to be constructed.

Samples with compositions near Zr_2Co_{11} have been synthesized for development of advanced magnetic materials [4]. In this work, JEOL JEM2010 and FEI Technai Osiris (scanning) transmission electron microscopes are used in the SAED and HREM experimental work. Simulated SAED patterns are calculated using SAED2.0 and experimental SAED patterns are measured using JECP/QSAED software [5].

Figure 1 shows a HREM image of the rhombohedral Zr_2Co_{11} phase with a corresponding SAED pattern as an insert. The image was taken with the incident electron beam along the [010] zone axis. The lattice parameters of the rhombohedral phase are a=0.48 nm and c=2.42 nm [2]. The observed spacing in the HREM image is d_{100}=0.42 nm and c=2.42 nm. A typical feature of the rhombohedral structure can be viewed as stacking layers along the c axis, which is marked as ABCABC in Figure 1. Simulation based on the theoretical predicated structural model is in a good agreement with the experimental results [3].

The orthorhombic Zr_2Co_{11} phase is an incommensurate modulated structure with a=0.476 nm, b=0.82 nm, c=0.275 nm and q^*=0.074c*, where $q^*=q_1a^*+q_2b^*+ q_3c^*$. Figure 2 shows a HREM image of the orthorhombic phase with a corresponding SAED pattern as an insert. The image was taken with the incident electron beam along the [010] zone axis. The image can be described as a network of perfect and deformed hexagons. Thus the hexagon can thus be viewed as a basic structural motif and the modification waves are formed by periodic transition of the perfect and deformed hexagons. A rectangular unit cell is marked to show an approximate unit cell (a=0.476 nm and $c\approx$3.58 nm) of the orthorhombic Zr_2Co_{11} phase. It shows that the structure projection contains two repeated units along the c axis.

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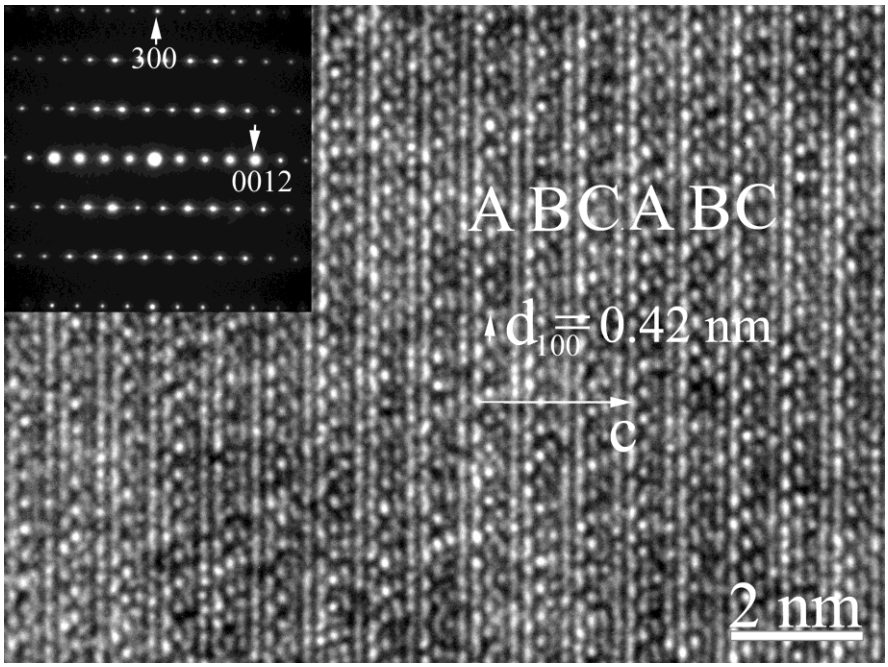

Figure 1. HREM image of the rhombohedral Zr_2Co_{11} phase and the corresponding SAED pattern.

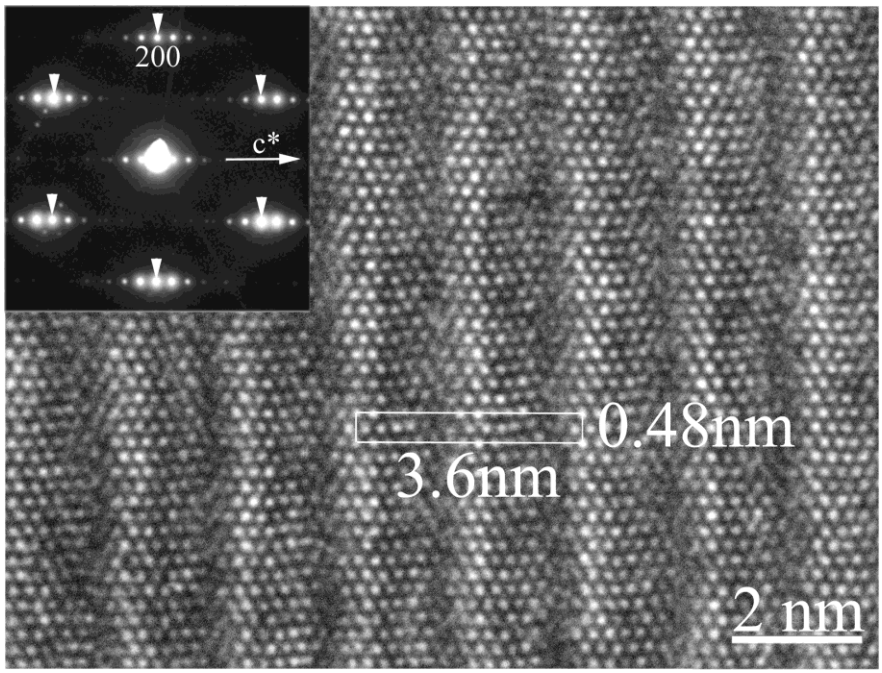

Figure 2. HREM image of the orthorhombic Zr_2Co_{11} phase and the corresponding SAED pattern.

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