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Imaging Dislocations in Complex Materials

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Deformation of metals and alloys by dislocations gliding between well-separated slip planes is understood but most crystal structures do not possess such simple geometric arrangements. Examples are the Laves phases with the AB_2 stoichiometry that are the most common class of intermetallic compounds and exist with ordered cubic, hexagonal and rhombohedral structures. These compounds are usually brittle at low temperatures and transformation from one structure to another is slow. Based on geometric and energetic grounds, a dislocation-based mechanism consisting of two shears in different directions on adjacent atomic planes has been proposed to explain both, deformation and phase transformations in this class of materials [1,2]. This paper reports direct observations, made by Z-contrast atomic resolution microscopy, of stacking faults and dislocation cores in Cr_2Hf that prove that a complex dislocation scheme does indeed operate in this ordered intermetallic material. Knowledge gained of the dislocation core structure will enable improved understanding of deformation mechanisms and phase transformation kinetics in this and other complex structures.

Figure 1 contains a schematic and micrograph of the hexangonal C14 variant of Cr_2Hf viewed along <11-20>. The structure is seen to consist of alternating layers of Cr and a buckled Hf-Cr-Hf layer. The Z-contrast image in Figure 2 shows a stacking fault in Cr_2Hf that comes in from the right about halfway up the image and terminates in the center of the micrograph at the dislocation core. The schematic shows the deduced core structure contains ‘extra’ Cr columns. It is the diffusion of Cr into and out of these columns that slows dislocation motion and makes this material brittle at low temperatures. A Laves phase transformation is illustrated in Figure 3 where a strip of the cubic C15 Laves phase has formed in the C14 structure by coordinated dislocation motion. The C15 structure results by shearing the C14 structure on alternate 3-layer stacks.

The motion of a single type of defect, a synchroShockley partial dislocation, is proposed to be responsible for shear phase transformations as well as three mechanisms of deformation: slip, twinning and stress-induced transformations. In this case, the kinetics of all four of these processes is controlled by the mobility of the complex dislocation core. Understanding the structure of the dislocation core and its influence on the ability of Laves phases to deform is central to designing alloys with optimized mechanical properties. In addition, these concepts can be extended to other crystal structures where the slip planes have more than one spacing.

References
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[3] This research was supported by the US Dept. of Energy under contract DE-AC05-00OR22725, the NSF contract DMR-9632524 and the US Air Force contract F33615-01-5214.

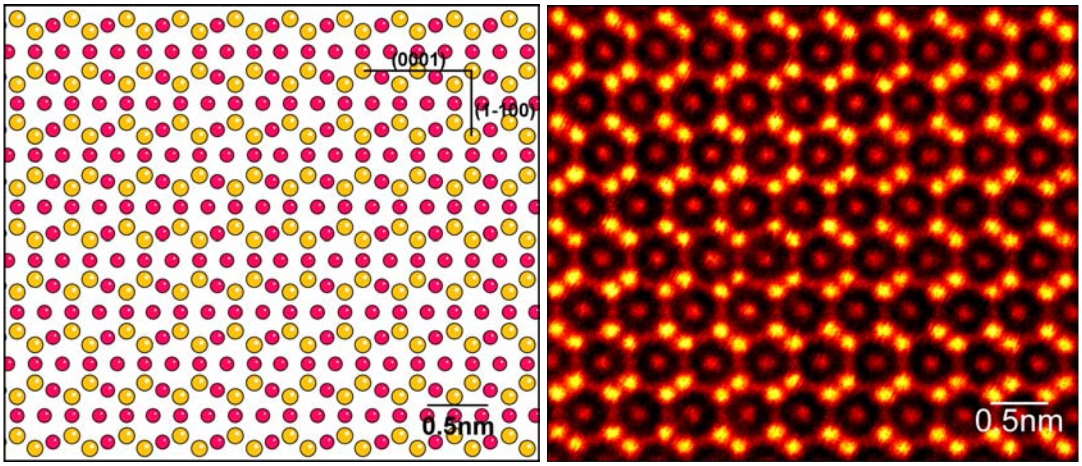

FIG. 1. (A) Schematic of the <11-20> projection of the C14 hexagonal Laves structure. The large atom sites are in yellow and the small atom sites are in red. (B) Z-contrast image of the <11-20> projection of Cr_2Hf. The bright features (yellow) are Hf columns and the less intense features (red) are Cr columns.

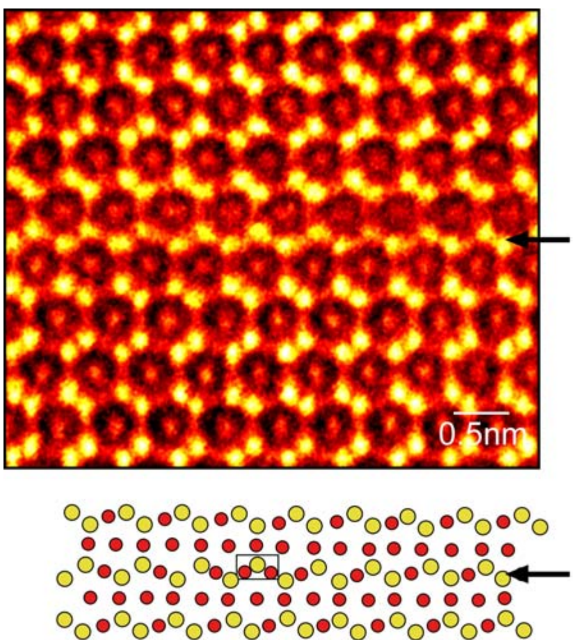

FIG. 2. Z-contrast image of the <11-20> projection of the a synchro-Shockley dislocation bounding a stacking fault in the C14 variant of the hexagonal Cr_2Hf Laves phase. The fault comes in from the right (indicated by arrows) and terminates at the dislocation core in the center of the image. The schematic below the image shows the deduced core structure.

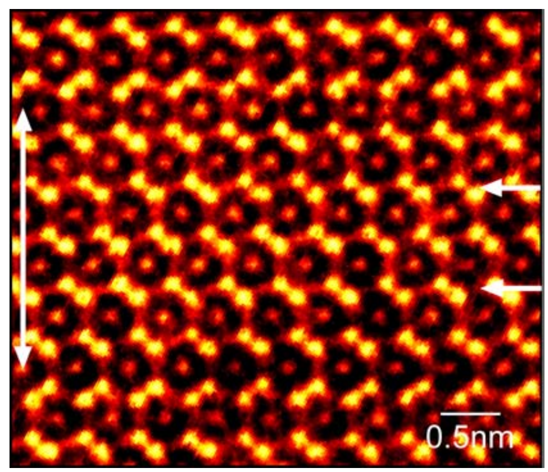

FIG. 3. Z-contrast image of the <11-20> projection of a faulted region of the C14 variant of the Cr_2Hf Laves phase. The region between the double arrow has the C15 cubic structure that could have formed by introducing two stacking faults (short arrows on the right).

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