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TEM Investigation on the Low Temperature Phase of HfV$_2$

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C15 Laves phase intermetallic compounds could be potential high temperature structural materials, in which C15 HfV$_2$ is particularly attractive$^1$. At room temperatures (RT), the C15 Laves phase has a fcc-based structure with a lattice parameter $a=7.4$ Å, as shown in Fig. 1. Sensitive specific heat measurements indicates that HfV$_2$ undergoes a structural transformation at 115 K, as shown in Fig. 2. The crystal structure of the low temperature (LT) phase of HfV$_2$ is not unambiguously clear, although some studies have been done$^2$-$^3$. A HfV$_2$ alloy was made by arc-melting. The alloy was homogenized at 1200°C for 120h. Preliminary study concentrated on selected area diffraction patterns (SAD) along different zone axes of C15 structure at 83 K, using a Philips CM 30 microscope with a liquid nitrogen cold stage.

$<100>_{C15}$ SAD at RT is shown in Fig. 3 (a). At 83 K, SADs along some $<100>_{C15}$ shows (100), (200), and (300) superlattice spots, as shown in Fig 3 (b), and SADs along other $<100>_{C15}$ indicates (110) and (200) superlattice spots, as shown in Fig. 3 (c). These SADs indicates that LT HfV$_2$ phase is not tetragonal based on the original cubic structure, i.e. not as claimed by Ref. 4. At 83 K, SAD along one [111]$_{C15}$ reveals no superlattice spots, i.e., being identical with $<111>$ SADs at RT. RT SAD along $<110>_{C15}$ is shown in Fig. 4 (a). At 83 K, two types of SADs along $<110>_{C15}$, as shown in Fig. 4 (b-c), reveals (111)/2, (113)/2, and (331)/2 superlattice spots. The appearance of (111)/2 superlattice spots means that the LT HfV$_2$ phase has larger lattice parameters, which is not consistent with Refs. 3-4. LT SADs along other zone axes, e.g., $<112>$, $<013>$, $<114>$, and $<332>$, reveal the same types, i.e., (111)/2, (113)/2, and (331)/2, superlattice spots.

Using a combination of these SADs, a tentative reciprocal lattice of LT HfV$_2$ is constructed, as shown in Fig. 5. It can be seen from Fig. 6 that the LT HfV$_2$ has an orthorhombic structure with three major axes being $a^*/[100]_{C15}$, $b^*/[011]_{C15}$, and $c^*/[011]_{C15}$, and with large lattice parameters$^4$. Further and detailed studies are under way, using a combination of CBED and synchrotron diffraction to determine unambiguously the crystal symmetry, lattice parameters, and atomic positions of the LT HfV$_2$.

References:
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FIG. 1 C15 crystal structure.
FIG. 2 Specific heat vs. temperature of HfV$_2$, indicating a structural transformation at 115.5 K.
FIG. 3 SAD along $<100>_{C15}$: (a) at RT, (b) at 83 K, and (c) at 83 K.
FIG. 4 SAD along $<110>_{C15}$: (a) at RT, (b) at 83 K, and (c) at 83 K.
FIG. 5 Reciprocal lattice of the LT HfV$_2$. 