Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Localized Rattling of Al atoms in $VAl_{10+\delta}$ DOUGLAS SAFARIK, Los Alamos National Laboratory, TOMASZ KLIMCZUK, Institute for Transuranium Elements, Karlsruhe, ANNA LLOBET, DARRIN BYLER, Los Alamos National Laboratory, EKHARD SALJE, Cambridge University — We have studied the localized rattling mode in the 'Einstein solid' $VAl_{10+\delta}$ using a suite of thermodynamic, transport, and neutron diffraction measurements. The rattling originates from Al atoms that occupy the large void within Z_{16} Friaf polyhedra, of which there are eight per unit cell in the $VAl_{10+\delta}$ structure. Our heat capacity, thermal expansion, and electrical resistivity data are all qualitatively consistent with a low-frequency harmonic vibration of the atom. However, our neutron diffraction data show that the rattling atom potential is better described as sixth-order, rather than harmonic. Using a single-site, sixth-order effective potential for the rattling atom, we can explain our thermodynamic, transport, and structural data, including the unusual temperature dependence of the elastic constants.

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Date submitted: 19 Nov 2010 Electronic form version 1.4