Quantum mechanics predicts unusual lattice dynamics of vanadium metal under high pressure

October 11 2007

A Swedish research team of Dr. Wei Luo & Professor Rajeev Ahuja and US team of Dr. Y. Ding & Prof. H.K. Mao have used theoretical calculations to understand a totally new type of high-pressure structural phase transition in vanadium. This phase was not found in earlier experiments for any element and compound. The findings are being published in this week's Net edition of the *Proceedings of the National Academy of Science*.

The relation between electronic structure and the crystallographic atomic arrangement is one of the fundamental questions in physics, geophysics and chemistry. Since the discovery of the atomic nature of matter and its periodic structure, this has remained as one of the main questions regarding the very foundation of solid systems.

Scientists at Carnegie's Geophysical Laboratory, USA and Uppsala University, Sweden have discovered a new type of phase transition - a change from one form to another-in vanadium, a metal that is commonly added to steel to make it harder and more durable.

Under extremely high pressures, pure vanadium crystals change their shape but do not take up less space as a result, unlike most other elements that undergo phase transitions. This work appeared in the February 23, 2007 issue of *Physical Review Letters*.

"Trying to understand why high-pressure vanadium uniquely has the record-high superconducting temperature of all known elements inspired us to study high-pressure structure of vanadium," said Dr. Wei Luo. "In present paper we have looked into the lattice dynamics of vanadium metal and it shows a very unusual behavior under pressure. A huge change in the electronic structure is driving force behind this unusual lattice dynamics. Moreover, our findings provide a new explanation for the continuous rising of superconducting temperature in high-pressure vanadium, and could lead us to the next breakthrough in superconducting materials."

Source: Uppsala University