Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Mechanical properties and electronic structure of Ta4AlC3[1]
SONGYOU WANG, MING XU, GANG YIN, LIANGYAO CHEN, State Key Laboratory of Advanced Photonic Materials and Devices, Department Optical Science and Engineering, Fudan University, Shanghai 200433, China, FENGCHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, YU JIA, School of Physics and Engineering, Zhengzhou University, Zhengzhou 450052, China — The mechanical properties and electronic structure of Ta4AlC3 have been studied using the first-principles calculations. Optimized structural parameters of the crystal structure and the calculated bulk modulus are in good agreement with the experimental data. The calculated bulk modulus reaches up to 262.40 GPa, which is the largest among all the known materials with MAX phases in the literature, the band-structure and the density of states suggest that Ta4AlC3 is metallic. Further analysis shows that the alternating stacks of relatively strong Ta-C bonding and weak Ta-Al bonding lead to the large bulk modulus of Ta4AlC3, but softening in shear.

[1]The work was supported by the NSF of China (Grant No. 60578046), the Shanghai Commission of Science and Technology (Grant No. 05PJ14016).

Songyou Wang
State Key Laboratory of Advanced Photonic Materials and Devices,
Department Optical Science and Engineering,
Fudan University, China

Date submitted: 02 Jan 2007 Electronic form version 1.4