Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Vibrational Behaviour of Metal Nanowires under Tensile stress[1]
YASEMIN SENGUN, Department of Physics, Istanbul Technical University, Maslak, 34469, Istanbul, Turkey, SONDAN DURUKANOGLU, Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, 34956 Istanbul, Turkey — We present results of calculations on vibrational density of states (VDOS) of a thin Cu nanowire with <100> axial orientation and discuss on the effect of axial strain. The calculations are performed using real space Green's function method with the force constant matrix extracted from the interaction potentials based on the embedded atom method. It is shown that the characteristics of the VDOS of a strain-free nanowire are quite distinctive compared to that of a bulk atom. Among the striking features of this type nanowire is the existence of high frequency modes above the top of the bulk spectrum. From an examination of VDOS of local atoms it is seen that the corner and core atoms are the primary moderators for the anomalous increase in low frequency and high frequency modes, respectively. We, additionally, find that while the high frequency band above the top of the bulk phonon shifts to even higher frequencies, the characteristics at low frequencies remains almost the same upon stretching the nanowire along the axial direction.

[1]This work is supported by TUBITAK under Grant No. 109T105.

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Date submitted: 30 Nov 2010 Electronic form version 1.4