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Report:

The aim of the experiment was the comparison of the vibrational DOS (VDOS) of Fe islands on Mo(110) with those of Fe islands on W(110). Correspondingly, two samples were prepared with a nominal coverage of about 4 ML Fe. The samples were then annealed for about 10 min at 700 K. This led to the formation of relaxed Fe islands (with the lattice constant of bcc Fe) on a pseudomorphic Fe monolayer on the surface. After preparation and characterization by LEED and Auger electron spectroscopy the samples were capped by about 3 nm of Ag for protection against oxidation in the subsequent ex-situ experiment.

Phonon spectra were taken at room temperature with an energy resolution of 3 meV, shown in the left panel of Fig. 1. From these spectra the VDOS was extracted, as shown on the right panel of Fig. 1. For comparison, the bulk density of states is shown in the top figure as dashed line (It was obtained from the bulk DOS calculated in a force-constant model and convoluted with the resolution function). The measured VDOS exhibits significant differences compared to the bulk DOS: a) At low energies below 15 meV one observes a significant enhancement of the measured VDOS and b) at high energies around 30 meV the measured VDOS is significantly reduced compared to the bulk DOS. Taking into account results from the recent beamtime SI-1097, we are able to interprete these observations and provide a semi-quantitative explanation. In that experiment we determined the VDOS of a single Fe monolayer on W(110) under UHV conditions. These results, briefly presented in the ESRF-flash 237 (17. Dec. 2004), were used to describe the vibrational properties of the monolayer here.

According to the structure of the sample, one expects two main contributions to the VDOS: That of the pseudomorphic monolayer and that of the relaxed islands. Correspondingly, both contributions were taken into account to simulate the VDOS in Fig. 1. For the contribution from the islands we have taken the DOS of bulk bcc Fe. It seems that the effect of the Ag capping layer is just a damping of the vibrational modes of the Fe. Therefore, in order to describe the measured DOS of the relaxed islands, $g(E)$, we have applied the model of a damped harmonic oscillator (DHO). At each energy E' of the calculated DOS $g_c(E)$ of bulk Fe, we have assumed an energy distribution given by $D(E', E)$:

$$g(E') = \int_0^\infty D(E', E)\, g_c(E)\, dE \quad \text{with} \quad D(E', E) = \frac{1}{\pi Q E'} \frac{1}{(E'/E - E/E')^2 + 1/Q^2}$$

In both cases a quality factor of $Q = 8$ led to a satisfactory simulation of the data. This damping describes the high-energy modes rather well. The enhancement of the low-energy modes is due to the contribution from the pseudomorphic monolayer. Both contributions are shown in the right panel of Fig. 1 as solid black lines and the sum of both is shown as solid red line. The relative fraction of both contributions reflects the relative fraction of the Fe in the monolayer and in the islands, respectively. We have tacitly taken the VDOS of the uncapped monolayer to describe the data here, also for the Mo(110) substrate. This is certainly a rough estimate. Therefore, additional data on capped monolayers on W(110) and Mo(110) have to be taken.

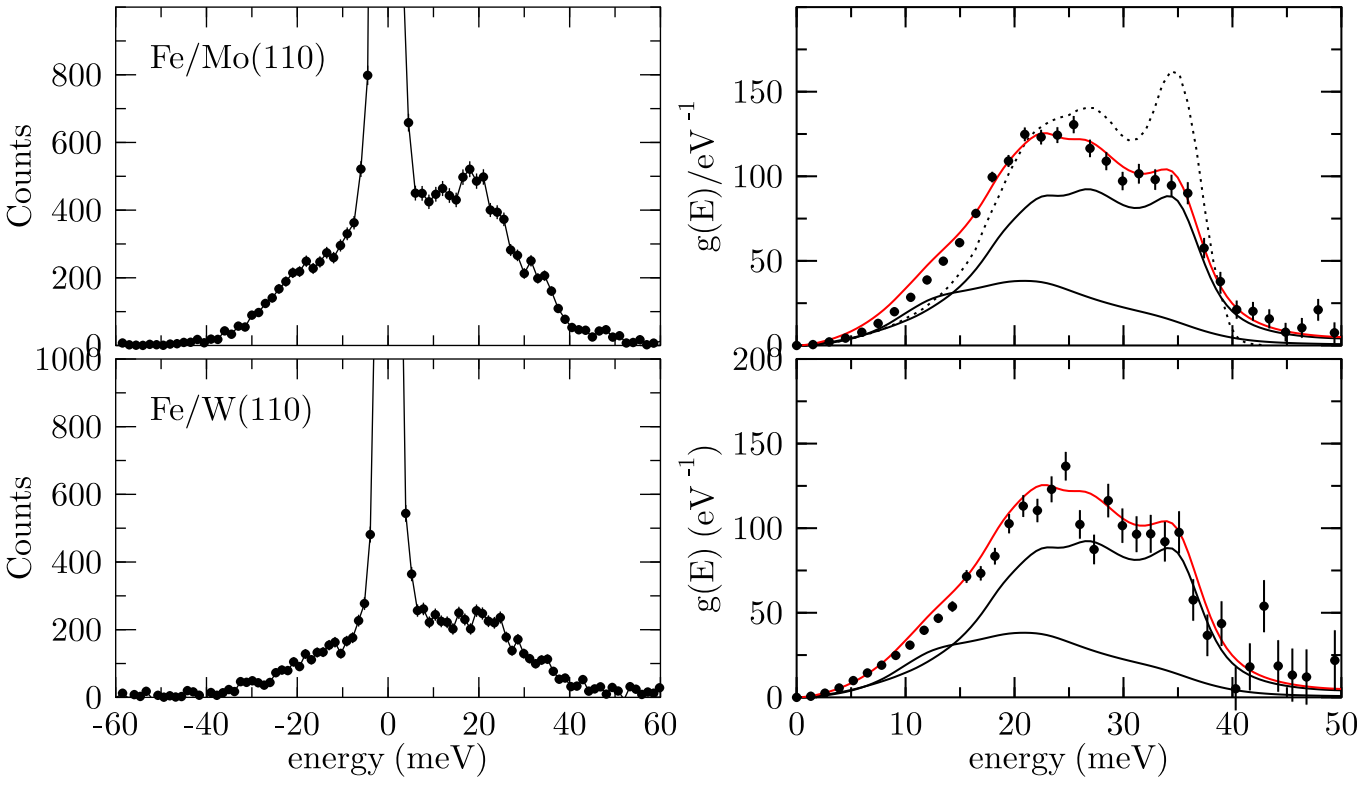

Fig. 1 : Phonon spectra (left column) and density of states (right column) of Ag-capped Fe islands on W(110) and Mo(110).