Notes

o.m8.o5 **Unusual multilayer $Al_3Li(100)$ surface alloy**.
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Al-Li alloys have attracted much attention due to their unique combination of low density and high stiffness. They are thus of special interest as potential light-weight materials in the aerospace industry. The metastable Al_3Li phase with $L1_2(Cu_3Au)$ structure is believed to play an important role in determining the mechanical properties of these alloys.

The surface structure of a metastable, multilayer Al-Li surface alloy formed by Li adsorption on Al(100) has been determined by quantitative analysis of low-energy electron diffraction measurements[1,2]. Adsorption of 0.5 monolayer (ML) Li leads to the formation of a c(2x2) structure in which Li atoms substitute every other Al atom in the first layer of the substrate[1]. The resulting structure is almost identical to the first layer in the $Al_3Li(100)$ surface. Adsorption of a further 0.5 ML Li leads to a further substitution of every other Al atom in the *third* layer of the substrate. This structure consists therefore of a mixed c(2x2)-Al/Li layer followed by an Al layer, followed by a second mixed c(2x2)-Al/Li layer[2,3]. However, contrary to expectation, the Li atoms in the third layer are not situated directly below the Li atoms in the first layer, as would be the case for the Al_3Li-$L1_2$ phase. Instead the Li atoms in the third layer are situated below the Al atoms of the first layer. Thus, the resulting structure corresponds to incipient growth of a $D0_3$ (Fe_3Al) phase.

This finding is in contrast to the results of ab initio calculations[4] which show that the *bulk* Al_3Li-$L1_2$ phase is of lower energy than a hypothetical bulk Al_3Li-$D0_3$ phase.

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