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Structure analysis of Na/Ge(111)-3X1 surface by tensor LEED

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Many adsorption experiments on semiconductor surfaces, especially on silicon surfaces have been done and a variety of superstructures have been observed. And surprisingly, the I-V curves of superstructures generated by different adsorbates are often almost identical. For example, the I-V curves of the 3X1 phases for the alkali metals adsorbed on Si(111) surfaces are similar. Such superstructures are due to adsorbate-driven substrate reconstruction. It is not difficult to expect that germanium surface, which has the same bulk structure, would undergo a similar behavior as the Si surface . And it has also been observed by previous workers. But the atomic structures of this adsorbed-metal induced reconstructions are not clearly understood. And this curiosity initiated this work.

In this work, the atomic structure of Na adsorbed Ge(111)-(1X3) surface was studied utilizing tensor LEED(Low Energy Electron Diffraction) analysis.

Tensor LEED is a perturbation method for calculating LEED I-V curves in which an initial reference structure is displaced. First it calculates changes in the t-matrix of the atom produced by displacing from their reference position as well as the diffraction intensity for the reference structure, which are used to do multi-dimensional optimization between experimental and theoretical I-V curves. With a suitable choice of reliability factor, we will present a set of atomic coordinates that gives a best fit between the two I-V curves.