Structure analysis of $FeSi_2$/Si(111) from LEED I-V curves calculation and ϕ-scan RHEED Patterson function pattern.

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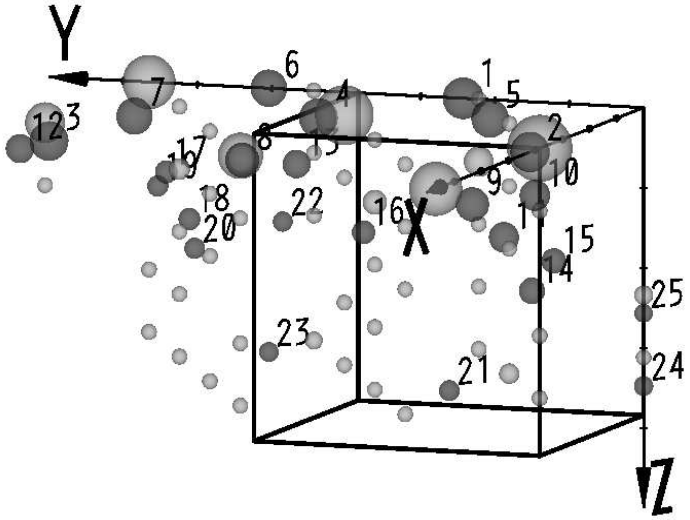
The atomic structure of iron silicide film grown epitaxially on the Si(111) surface has been analyzed by LEED I-V curves calculation and three dimensional Patterson function calculation using LEED and RHEED intensity. We have prepared iron silicide surface by solid phase epitaxy method by deposition of 2 ML of Fe on the Si(111) 7x7 and annealing at 500 C° to obtain 2x2 terminated γ-$FeSi_2$ phase. LEED I-V curves analysis involves trial-and-error procedure and we have faulted to solve the structure by this technique. Because that the direct Patterson function calculation was suggested.



ϕ-scan RHEED pattern conversion from screen -> k-space -> screen has been applied for receiving regular distribution of RHEED intensities and, therefore, calculate the three dimensional Patterson function (Fig. 1). The convoluted model of iron silicide structure from Patterson function spots has two silicide layers faulted to each other. There are three Si adatoms relaxed to the Fe plane form the 2x2 Si terminated superstructure with Si atoms on the H_3 site.

Figure 1 – 3D Patterson function distribution derived from RHEED intensities.

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