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Raman study of tetragonal tungsten disilicide

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Abstract

After a brief report of recent WSi_2 Raman results on the band assignment and thermal behavior of the WSi_2 lines obtained for both a single crystal and a thin film, a calculation of vibrational frequencies and normal coordinates at the zone center is presented. The first results show good agreement between observed and calculated frequencies, and confirm our previous description of vibrational modes. The corresponding force constants relative to Si–Si and W–Si bonds are found to be different while the bond lengths are very close. The present results will be used in future calculations at the zone boundary.

1. Introduction

Transition metal silicides have been the topic of numerous studies investigating their properties [1,2], but very few are related to their vibrational properties, in particular for tungsten disilicide.

Raman and IR spectroscopic studies of WSi_2 already reported in the literature have been performed on thin films at room temperature [3–6]. The purpose of our WSi_2 Raman study is to evidence spectral features of the compound in both the crystal and film states in a broad temperature range. Such spectral data can be directly used for in-situ Raman characterization of WSi_2 films during the deposition process.

Our recent Raman results about the band assignment and the temperature dependence of the WSi_2 lines of single crystal and thin film [7] are recalled in the first part of this paper. Then, a calculation of vibrational frequencies and normal coordinates of WSi_2 at the zone center is reported. This calculation allows one to precisely determine the potential energy distribution in WSi_2 and the atomic displacements in each vibrational mode.

2. Structure and experimental procedure

2.1. Crystal structure

WSi_2 crystallizes in the body-centered tetragonal structure with two formula units per unit cell (C11b structure, space group I4/mmm or D_{4h}^{17}) [8] (Fig. 1a). The lattice constants are $a = 3.213$ Å and $c = 7.830$ Å. The W–Si–Si sequence of atoms aligned along the [001] direction is considered for the WSi_2 lattice vibration study [7]. All the atoms are ten-fold coordinated with a pseudo-hexagonal arrangement in

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