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The calculation of positron lifetime in Ni_3Al alloy*

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Abstract. Superposed-neutral-atom model and the finite-difference method (SNA-FD) are used to calculate the positron lifetime of different sizes and types of vacancy clusters in Ni_3Al alloy. The calculated positron bulk lifetime in Ni_3Al agrees well with the experimental results mentioned in literatures. The positron lifetimes of vacancy clusters with the same amount of vacancy but different components are also calculated. The results show that the positron lifetime is different when its components are different. The positron lifetimes of vacancy clusters with a single element but different sizes are also calculated. The result shows that the positron lifetime is almost a constant when its component is only Al vacancy, but the positron lifetime will increase at first and trend to be a constant when its component is only Ni vacancy.

Introduction

The intermetallic compound Ni_3Al has the crystal structure LI2. This structure is an important phase for strengthening the materials. Ni_3Al -based alloys for structural applications have been an active field of research in material science for over two decades [1,2]. Positron annihilation is an important method in the study of defects in solids. It can produce “fingerprints” of vacancy type defects of various sizes and structures [3,4,5]. Theoretical calculations of positron states and the annihilation characteristics play an important role in the interpretation of experiments employing positron techniques. Firstly, it can give a realistic description of the positron distribution and energetics in the solid. Secondly, it provides predictions for the positron annihilation characteristics.

The methods

The SNA-FD method is extensively used in the positron calculations. An effective positron potential is first constructed followed by solution of the positron schrodinger equation. The annihilation characteristics can then be calculated from the positron and electron densities and /or wave functions. When calculating lifetimes it is essential to include the effects of electro-positron correlations which lead to an enhancement of the annihilation rate due to the pile-up of electrons around the positron. It is common to divide the electrons in the system into different classes, i.e. valence-band, d-band and core electrons, which allows different descriptions of the correlation effects to be employed for each class [6,7].

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