HRTEM images simulation of Al-Mg-Si GP Zone

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1. Introduction

Al-Mg-Si alloys are an important group of alloys that are widely used in both cast and wrought form. The alloys are age hardenable. The age-hardening response of the alloys is very significant and hence control of precipitation during heat treatment is critical for attaining optimal alloy performance. In generally, the precipitation sequence was summarized as following: clusters of Si atoms→GP zones→ β'' → β' → β Mg_2Si. The formation of GP zones is the initiative stage of precipitation. But some of the atomic structure of GP zones is unknown, because the size of these zones is very fine (usually several nano-meter or even more small). Simulated HRTEM image is a powerful technique to be used to study the unknown structure. We can construct some possible atomic structural model in advance, then simulated HRTEM images of these models and compared with experimental images. By the compared results, some unknown structure can be confirmed.

2. Construction of models and simulation condition

In study, we construct the following models:

a. One line of Mg or Si atoms were placed at the fcc Al matrix's lattice points, and formation vertical single layer GP zone, as shown in Fig.1(a).

b. Two lines of Mg or Si atoms were placed at the fcc Al matrix's lattice points, formation two lines and two rows GP zone, as shown in Fig.1(b).

c. Several Mg or Si atoms of two layers were places at the fcc Al matrix's lattice points, formation closed GP zone, as shown in Fig.1(c).

d. One slice of GP zones in Fig.1(c) were embedded in Al matrix, simulated the images of various thickness of Al matrix and GP zone in different position which the GP zones were placed the top, middle and bottom of Al matrix, as shown in Fig.2.

120Kv accelerated voltage was adopted. And the 7×7 is as the basis unit-cells, one slice is 0.405nm.

3. Simulated results

Fig.3 (a), (b) and (c) shows the HRTEM simulation images of vertical single layer (model a) corresponding to Mg-rich GP zones, Si-rich GP zone and Mg-Si GP zone, respectively. Mg-rich or Si-rich is that Mg atoms or Si atoms replaced all the atoms in GP zone. Mg-Si GP zone means that one layer is Mg atoms and the second layer is Si atoms in GP zone. These images indicated that Mg-rich GP zone and Si-rich GP zone have inverse contrast. Fig.4 shows the simulated HRTEM images of different thickness corresponding to model b. Fig.5 shows the simulated HRTEM images of different Al thickness corresponding to Fig.2 (a), which the model of GP zone is as shown in Fig.1(c) and GP zone located on the top of Al matrix. Simulated results in Fig.6 corresponding to Fig.2(b), which GP zone was located in the middle of Al matrix. Simulated HRTEM images in Fig.7 corresponding to the Fig.2(c), which GP zone was located on the bottom of Al matrix. From these results, it indicated that GP zone images could be observed only in Fig.5 , no clear GP images were observed when GP zone was located in the middle and on the bottom of Al matrix. The simulated images of Mg-rich and Si-rich corresponding to Fig.2 also show the

same results, only the GP zone can be observed when GP zone located on the top of Al matrix.

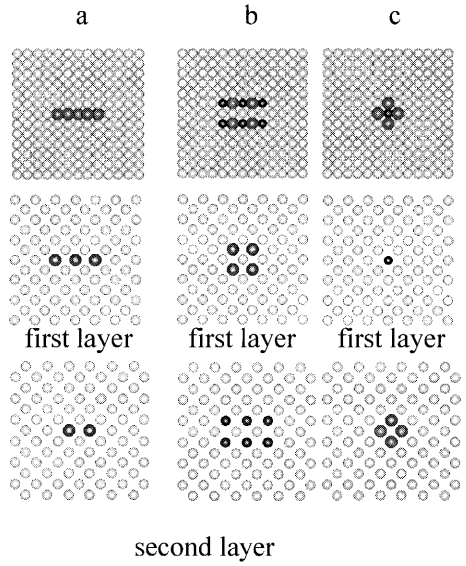

Fig.1 The models were constructed. White spheres represent Al atoms, large black ones represent Mg atoms; and small black ones represent Si atoms.
a. vertical single line GP zone
b. vertical two lines GP zone
c. closed GP zone

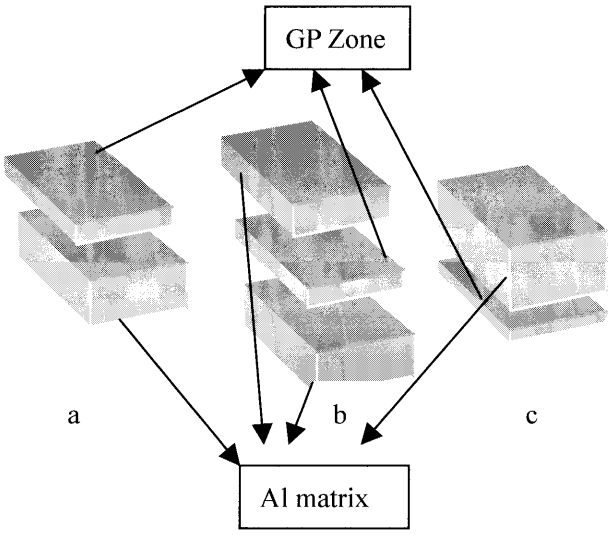

Fig.2 The models of two phases simulation.
a. GP zone on the top of Al matrix
b. GP zone in the middle of Al matrix
c. GP zone on the bottom of Al matrix.

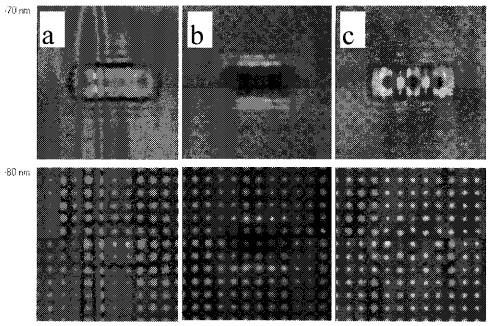

Fig.3 Simulated HRTEM images of model a.
a. Mg-rich GP zone
b. b. Si-rich GP zone
c. c. Mg-Si GP zone.

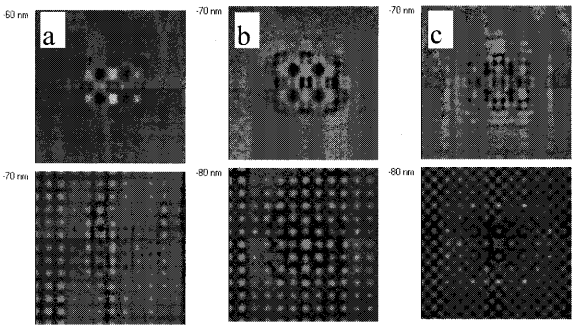

Fig.4 Simulated HRTEM images of model b.
a. The thickness is 10 slice
b. The thickness is 50 slice
c. The thickness is 100 slice

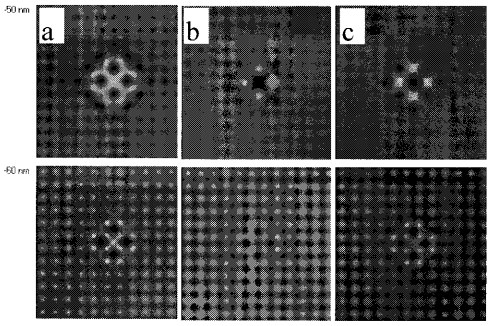

Fig.5 Simulated HRTEM images of Fig.2 (a).
b. The thickness is 10 slice
b. The thickness is 50 slice
c. The thickness is 150 slice

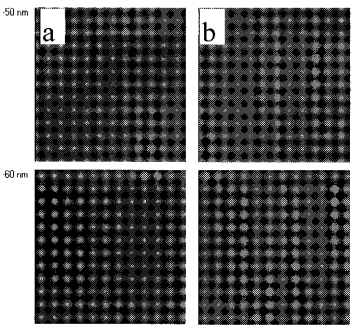

Fig.6 Simulated HRTEM images of Fig.2 (b).
a. The thickness is 20 slice
b. The thickness is 100 slice

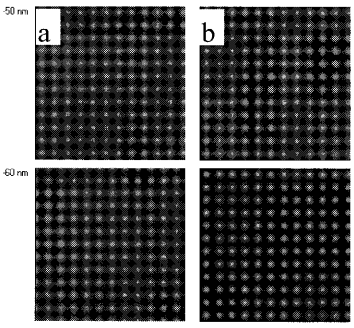

Fig.7 Simulated HRTEM images of Fig.2 (c).
a.The thickness is 20 slice
b. The thickness is 100 slice