RCI Simulation for EUV spectra from Sn ions

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Abstract. Using the relativistic-configuration-interaction atomic structure code, RCI simulations for EUV spectra from Sn$^{10+}$, Sn$^{11+}$ and Sn$^{12+}$ ions are carried out, where it is assumed that each ion is embedded in a LTE plasma with the electron temperature of 30 eV. To make clear assignment of the measured spectra, the value of the excitation energy limit, which is introduced to limit the number of excited states in the simulation, is changed to see the excitation-energy-limit dependence of the spectral shape. The simulated spectra are obtained as a superposition of line intensities due to all possible transitions between two states whose excitation energy from the ground state is lower than the excitation energy limit assumed. The RCI simulated spectra are compared to the spectra measured with the charge-exchange-collision experiment in which a rare gas such as Xe or He as a target is bombarded by a charge-selected tin ion. Applicability of the LTE model to a decay model in the charge exchange collision experiment is also discussed.

1. Introduction

In developing next-generation lithography machines, one of the most important parts of them is to make EUV light sources which can emit strong lines in a narrow wavelength region around 13.5 nm. Recently, tin has become of major interest because of the strong and narrow spectral feature in the wavelength region near 13.5 nm observed. Shimada et al have measured the EUV spectra from tin plasmas produced by high-power laser irradiation [1], where only a broad single peak in the wavelength region around 13.5 nm has been observed. This shows that the spectra emitted from the laser produced plasmas consist of a large number of lines emitted from various tin ions. Moreover the shape in the spectra observed is deeply dependent on the plasma conditions used in the experiment. Therefore in the analysis of the spectra from tin plasmas, reliable spectral data from individual tin ions with the definite charge state are needed. Along this line Tanuma et al [2] have carried out systematic measurements of the EUV spectra from each Sn$^{(q-1)+}$ (q=5-15) ions through the charge-exchange collisions between a charge-selected Sn$^{q+}$ ion and a rare gas such as helium or xenon. In the analysis of their measured spectra it is required to deal with a decay model for each tin ion in a higher excited state produced after the charge exchange collision. However it is difficult to pursue all decay paths in a multi-electron atomic system completely because so many decay paths exist due to many multiplet states arising from configurations constructed from one-electron functions having principal quantum numbers more than three in the atomic systems under consideration. After the successive decays in the
ion produced by the charge exchange collision, most decay paths pass through a limited number of lower excited states which play a dominant role in emitting strong lines of the spectra observed. This means that the lines emitted in the charge exchange collision are largely dependent on the decay route so that the relative population among the lower excited states in a decay model is considered to be in proportion to the number of decay paths which pass through each state. On the other hand, in a simple local thermodynamic equilibrium (LTE) plasma model, the relative population in each excited state with respect to the ground state in an ion embedded in a plasma is calculated easily by use of the Boltzmann law in classical statistical mechanics. This suggests that if a simulated spectrum from a tin ion using the LTE model agrees with the experiment, the relative population among lower excited states in the decay model can well be estimated with the Boltzmann law. Even if discrepancy between the simulated spectra with the LTE model and experiment is observed, it is possible to look into the decay paths in more detail from it because emission lines due to transitions from all the excited states are used to construct the spectra in the LTE model. So it is interesting to use the LTE model in the analysis of the spectra measured with the charge exchange collision. Although the spectra measured by Tanuma et al. are not resolved so as to be able to distinguish individual lines, if one focuses on the feature of the spectral shape, one can simulate the experimental spectra having a characteristic spectral shape by superposing intensities of all lines with the LTE model.

In this work, using the RCI atomic structure code [3,4], we simulate EUV spectra from each tin ion based on the LTE plasma model. Comparison of the spectra between theoretical RCI simulations with the experiment by Tanuma et al is made to see the accuracy of the RCI results.

2. Method of Simulation

In the present RCI calculation for energies and wave functions in each tin ion, both real and virtual DF functions from 1s up to 5f_{7/2} form a basis set which is used to construct CSF’s. A total wave function is expressed as a superposition of CSF’s. When constructing CSF’s, all possible one-electron and two-electron excitations from the valence 4d orbital are taken into account.

In obtaining the simulated spectra for a particular ion, wavelength region is divided into narrow intervals of 0.1 nm and the line intensity for each wavelength interval is then obtained as a sum of line intensities for the transitions whose wavelengths are included in this interval. Here we assume that each ion is embedded in a LTE plasma with the electron temperature of 30eV so that relative population in all excited states with respect to the population in the ground state in the ion is calculated by use of the Boltzmann law. Each line intensity is obtained as a product of Einstein’s A-coefficient and a population of an upper state from which the transition occurs. In order to make clear assignment of the spectra measured, we carry out simulations for the spectra from all tin ions considered by taking three values of 100 eV, 150 eV and 200 eV as the maximum value of the excitation energy. When the magnitude of the maximum excitation energy increases, new lines due to the transitions from higher excited states allowed by the larger value of the excitation energy appear in the spectra so that one can assign these lines as a result of transitions related to the higher excited states newly taken into account.

3. Results

Tanuma et al. have used two kinds of neutral rare gases, that is, helium and xenon, as a target atom to measure the EUV spectra from each tin ion as a projectile. Here we pick the spectra from Sn^{10+}, Sn^{11+} and Sn^{12+} because it is found from the analysis of the spectra from the laser-produced tin plasmas with the hydrodynamic code [1] that the abundance of these ions in the plasmas is much larger than that of other ions.

In figure 1 (a), (b) and (c), RCI simulated spectra for Sn^{10+}, Sn^{11+} and Sn^{12+} with the excitation-energy limit of 150 eV are compared with corresponding spectra measured by Tanuma et al. It is found from figure 1(a) for Sn^{10+} that the spectral feature consisting of two broad peaks in the wavelength region between 12.5 nm and 17 nm is similar to that of the experimental one although both
Figure 1. Comparison of RCI simulated spectra with the excitation-energy limit of 150 eV from (a) Sn$^{10+}$; (b) Sn$^{11+}$ and (c) Sn$^{12+}$ with the spectra from corresponding ions measured by Tanuma et al.
peak positions in the RCI spectra are about 0.5 nm shifted to the shorter wavelength side compared to the experiment. In figure 1(b) for Sn$^{11+}$ one sees many strong lines spread over the wavelength region between 12 nm and 15.5 nm in the RCI spectrum, whereas the two spectra measured consist of a single narrow peak around 13.5 nm and comb-shaped four lines distributed between 14 nm and 15 nm. On the other hand it is seen from the figure 1(c) for Sn$^{12+}$ that the spectral feature of the narrow peak around 13.5 nm in the measured spectra is well reproduced with the RCI simulation. Discrepancy of the spectra in the wavelength region longer than 14 nm between the RCI result and the experiment shows that emissions from specific excited states along the decay paths in the charge-exchange collision are not adequately selected with the LTE model.

4. Discussion

It is interesting to discuss whether our theoretical model for each tin ion embedded in a LTE plasma is adequate to describe the experimental situation of the charge-exchange collision, or not. A single band-like peak observed in the spectra from the ions mainly arises from mixture of lines due to the 4f-4d resonance transitions and the 5p-4d transitions, in which only lower excited states having the 4f and 5p electrons contribute to the spectra in this wavelength region. Large population in these lower excited states can constantly be produced in a LTE plasma. On the other hand, strong lines with the 4f-4d and 5p-4d transitions could also be observed in the charge-exchange-collision experiment because it is considered that most decays for the ions in a higher excited state produced after the collision reach the lower excited states which produce these lines. However, the measured spectra always contain continuous small peaks in longer wavelength region more than 16 nm. This feature of the spectra cannot be reproduced by the present RCI simulation. So these peaks seem to appear with a large number of lines due to transitions between higher excited states than those taken into account in the present simulation.

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