SECONDARY PROCESSES IN GASEOUS BORON ACCOMPANYING THE CASCADE DECAY OF THE 1S-VACANCY

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We employ the Monte-Carlo technique to simulate the processes in gaseous boron initiated by 1s-photoionization of boron atoms. The processes of excitations/ionizations of atoms by photons and electrons emitted by the neighboring decaying atoms are considered. It is found that the medium effect becomes noticeable at atomic densities of about $2.5\times10^{20}m^{-3}$

Introduction

Cascading decay of an atomic inner-shell vacancy is a fundamental atomic process leading to multiple ionization and emission of complex multi-component electron spectra and photon spectra. At the first decay steps when the decaying atom emits photons and electrons of great energies, these may well cause the ionization of neighboring atoms and thus trigger new cascades. Although the initial-inner-vacancy cascades are being studied since sixties, the effect of the surrounding media has not yet been addressed.

In this work we use the Monte Carlo (MC) technique to simulate the processes initiated by photoionization of the boron atoms in gas phase at various pressures in the interaction zone.

Method of calculation

The interaction zone is a cylinder of a 0.1 cm radius. A narrow primary photon beam ionizes the atoms on the cylinder axis. Photons and electrons produced by the decay processes are surveyed as they propagate through the media: the photons can be absorbed, the electrons scattered elastically or inelastically. Absorption of a photons or inelastic scattering of an electron produce excited atomic states which may start to decay themselves.

The MC code is written in Java. It accesses a relational database which contains the atomic structure data like cross sections and transition matrix elements. It makes use of the object relational mapping tool Hibernate and the Spring framework [1,2].

The following processes are considered in our simulations:

- all radiative and radiationless decay pathways for each initial and intermediate ionic state,
- photoionization by primary and cascade-produced photons,
- excitation/ionization of atoms by cascade-produced electrons,
- the processes of additional monopole excitation/ionization upon photo- and electron-impact ionization,
- elastic scattering of electrons

The quantities needed for the MC simulations are then radiative and radiationless (Auger, Coster-Kronig) transition rates, photoionization cross sections, electron impact excitation and ionization cross sections, elastic electron scattering cross sections, shake up and shake off probabilities due to photo- and electron impact ionization.

All the above values (except elastic electron scattering cross sections [3]) are calculated in configuration-average approximation with the Pauli-Fock wave functions for the core and continuous spectrum states. Calculated photoionization and electron impact ionization cross sections are presented in Fig. 1, 2, where they are compared with available data from literature.

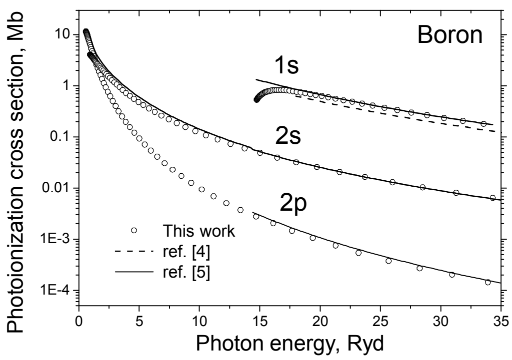

Fig.1. Partial photoionization cross sections for the boron atom

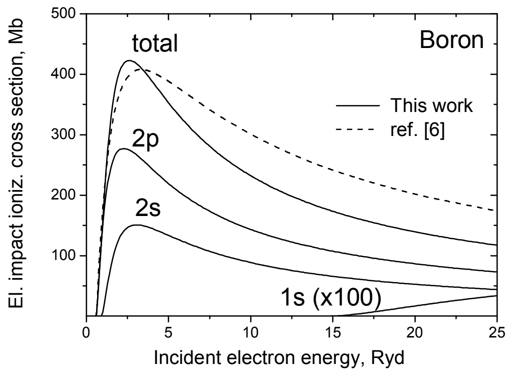

Fig.2. Partial and total electron impact ionization cross sections for the boron atom

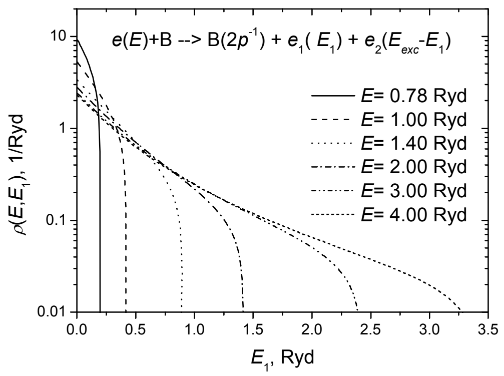

Fig.3. Densities of probabilities for one of the electrons to have an energy E_1 upon 2p electron impact ionization of B

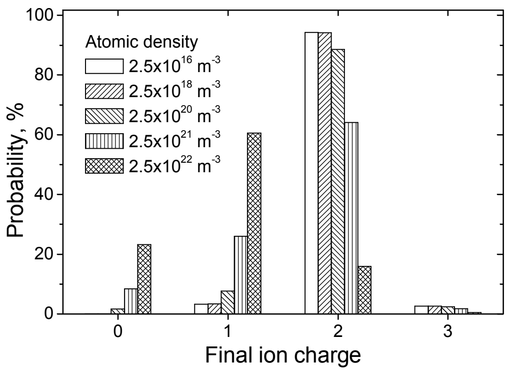

Fig.4. Calculated final B^{i+} ion charge spectra upon photoionization of gaseous boron with 20 Ryd photons at various atomic densities in the interaction zone.

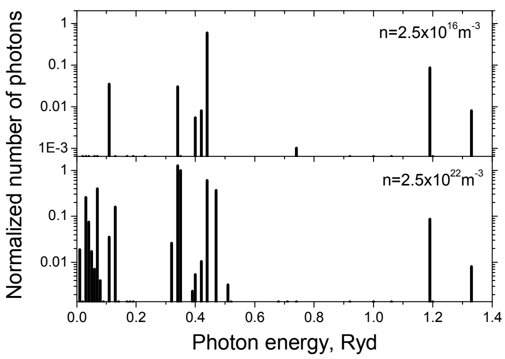

Fig.5. Calculated photon emission spectra upon photoionization of gaseous boron with 20 Ryd photons at low and high atomic densities in the interaction zone.

Upon *nl*-subshell electron impact ionization at the incident electron energy E two electrons in the final state share the excess energy $E_s = E - I_{nl}$. The mode of this energy sharing is crucial for realistic MC simulations. We calculated the densities of probabilities $\rho(E,E_1)$ for one of the electrons to have an energy E_1 upon electron impact ionization at an energy E (the other one has then $E_2=E_s-E_1$). The results in the case of 2p electron impact 2*p*-ionization at various incident electron energies are presented in Fig.3. One can see that the energy sharing is very asymmetric.

We found a simple two-parameter formula which interpolates the distributions $\rho(E,E_1)$ for 2*p* and 2*s* electron impact ionizations.

Results and discussion

Fig.4. shows calculated final-ion-charge distributions at various atomic densities in the interaction zone.

Low-energy photon emission spectra and electron spectra from the interaction zone at low and high atomic densities are shown in Figs. 5 and 6.

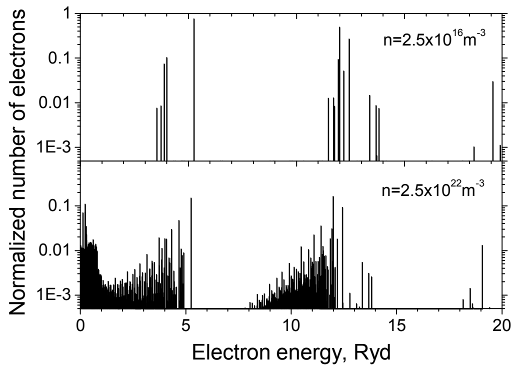

Fig.6. Calculated electron spectra upon photoionization of gaseous boron with 20 Ryd photons at low and high atomic densities in the interaction zone.

One can see from Figs.4-6 that the ion-yield, photon and electron cascade spectra are sensitive to the environment. As can be seen from Fig.4 the effect is significant starting from the atomic density of about $10^{20}m^{-3}$. Inclusion of the medium effect is obligatory in theoretical description of the decay cascades in dense samples, like liquids and solids.

References

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