iNCLUSION OF shell eFFECTS IN tHE sTATISTICAL MODEL OF FREE IONS

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The characteristics of free positive ions have been studied with a semiclassical method, based on the Thomas-Fermi statistical model. An efficient method has been proposed to include of the discretness of the electronic spectrum and the calculation of a shell correction to the number of states by the statistical model in the case of the strong irregularity of the correction. The calculation of the free-ion ionization potentials within this approach reproduces the “sawtooth” dependence of these potentials on the ion charge and appreciably improves the description of the experimental data by the statistical model.

Shell effects are due to the discretness of the spectrum of bound electrons in atomic systems (atom, ion, atomic cell of matter). These effects were successfully taken into account in [1], [2] for the calculation of ion ionization potentials in statistical model of a hot plasma. The semiclassical method used in those works is based on the assumption that shell effects smoothly change physical quantities. However, this assumption is invalid for zero temperature. In this case, shell effects are manifested in sharp dependences, e.g. a sawtooth dependence (similar to the dependence of atomic ionization potentials on the atomic number) of ion ionization potentials on the ion charge or a casplike dependence (similar to atomic volume curve [3]).

In this work, we propose a generalization of the semiclassical method that removes the indicated restriction. The ion ionization potentials calculated by the generalized method exibit the mentioned sharp dependences and are much closer to the experimental data.

References

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