

Interatomic potentials, atom energy and screening constants

Alexander N Zinoviev

Ioffe Institute St Petersburg, Russia

Simple formulae for estimating atom energy (the electron subsystem energy of atom) and screening constant have been proposed. The formula for the screening constant fits well experimental data on interaction potentials. Quantitative description of the experiment for the effect of electronic screening on the nuclear synthesis reaction cross-section for the D+/-D system has been obtained. A conclusion has been made that the differences between the measured cross-sections and their theoretically predicted values which take place in more complicated cases of nuclear synthesis reactions are not caused by uncertainties in the knowledge of interatomic potentials. The interatomic potential determines the nuclear stopping power in materials. Experimental data prove that the approach of determining interatomic potentials from quasielastic scattering can be successfully used. Experimental data on the scattering of atomic particles were analyzed and an analytical potential form was proposed as the best fit of the available experimental data. It is shown that Application of any universal potential is limited to internuclear distances $R < 7 a_f$ (a_f is the Firsov length). The paper discusses pair-specific interatomic potentials determined both experimentally and by density-functional theory simulations with the DMol approach to choosing basic wave functions. The interatomic potentials calculated using the DMol approach demonstrate an unexpectedly good agreement with experimental data. Differences are mainly observed for heavy atom systems, which suggests that they can be improved by extending the basis set and more accurately considering the relativistic effects. These data are recommended for modeling collision cascades in ion-solid collisions. New methods to obtain potential parameters from rainbow scattering features in the atom-metal surface collisions are discussed. Obtained results differ strongly from the known binary potential models. This difference is explained by the influence of interaction of the projectile with metal electrons. Observed patterns of black-body radiation.

Biography

Alexander Zinoviev has his expertise in atomic, plasma and nuclear physics. He completed his PhD at the age of 31 and later, in 1992, got the status of Dr Habil from Ioffe Institute in St. Petersburg. He has been selected as a head of the lab of atomic collision in solids. He is a coordinator of the Atomic Physics Research at Ioffe Institute.

zinoviev@inprof.ioffe.ru