ThuPE14

Simulation of diatomic gas-wall interaction and accommodation coefficients for Negative Ion Sources and accelerators

E. Sartori*[a], G. Serianni[a]

[a]*Consorzio RFX, Euratom-ENEA association, Padova, Italy*
**emanuele.sartori@igi.cnr.it*

Particle-wall interactions determine in different ways the operating conditions of plasma sources, ion accelerators and beams operating in vacuum. A strong contribution to gas heating in plasma source is given by ion neutralization at walls; beam losses and stray particle production – particularly detrimental for high current negative ion systems such as beam sources for fusion – are caused by collisional processes with residual gas. The gas density profile is determined by the scattering of neutral particles at the walls. The modeling of realistic gas flows in vacuum involves some assumption on the gas-surface interaction, concerning the features of inelastic scattering, momentum and energy exchange, and the angular distribution of scattered particles. The influence of the accommodation coefficient on efficiency losses in the case of accelerators for fusion was shown in the past [1]. The study of such gas-wall interactions, scattering and accommodation parameters, can be performed by use of Molecular Dynamics (MD) techniques.

This paper shows that MD studies at the nano-scale can provide Momentum Accommodation Coefficient (MAC) and Energy Accommodation Coefficient (EAC), which in non-isothermal flows (such as the neutral gas in the accelerator, coming from the plasma source) affect the gas density gradients. For ideal surfaces the computation also provides the angular distribution of scattered particles. Classical MD method has been applied to the case of diatomic molecules. Single collision events, against a frozen wall or a fully thermal lattice, have been simulated using probe molecules. The two wall modeling approximations and data from literature are compared to verify the numerical results.