Scattering kernels analysis based on molecular dynamics computation results

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Molecular dynamics trajectory computation results for hydrogen on graphite surface were compared with Maxwell, Epstein and Cercignani-Lampis scattering kernels and analyzed.

It was obtained that tangential momentum and energy accommodation coefficients significantly depend on initial velocity of inlet molecule. At low surface temperatures (87K) one part of the inlet molecules physically adsorbed on graphite, some time located near the surface and after it desorbed. The velocity distribution of this part of molecules can be approximated by perfect accommodation. Another part of molecules was scattered without adsorption with some non-zero accommodation coefficients.

Analysis of known scattering kernels shows that Epstein kernel is more suitable than Maxwell and Cercignani-Lampis kernels for hydrogen on graphite. But quantitatively the computed velocity distribution functions differ significantly from simple diffuse-specular form of Epstein model.

Based on obtained in trajectory MD computation results a new scattering kernel was proposed as a combination of Epstein and Cercignani-Lampis models. The main advantage of proposed kernel in comparison with numerical approximation of computed data is analytical integrability and determination of momentum and energy flows in an explicit form. It was showed that proposed kernel is in a good agreement with trajectory computational results.

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