Impact induced multifragmentation of fullerene on gold: experimentally motivated molecular dynamics simulations

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Postcollision multifragmentation phenomena for the impact of C_{60}^{-} ions on gold and nickel was recently observed over a wide range (80-900 eV) of impact energies [1]. In order to gain a deeper insight into the microscopic dynamics of the fullerene multifragmentation processes, we have carried out molecular dynamics (MD) simulations of C_{60} single impacts with an Au (001) target under nearly the same initial conditions and scattering parameters as the experimental ones. Both, near threshold (80-120 eV) and full multifragmentation (higher impact energies) regimes were studied. In the near threshold energies we have studied the dynamics of both intact scattering and onset of multifragmentation events.

The results of our simulations are in relatively good agreement with the near-threshold behavior observed in the experiment for a similar range of impact energies. The calculated multifragmentation yield curve exhibits a threshold behavior at 90-100eV as compared with the 80-100 eV experimental value. A constant relative energy loss for the intact scattered C_{60} was found, as a function of impact energy for the 80-160 eV range, for different incident angles (Θ_i=22, 63 deg).

The main characteristics of a postcollision multifragmentation event (300 eV) are reproduced in the calculations and found to be in qualitative and nearly quantitative agreement with the experimental results. It appears that from the moment of the initial impact induced deformation and till actual fragmentation, the deformed fullerene undergoes a sequence of structural transformations characterized by a gradual reduction in the level of coordination of the carbon atoms (decreasing connectivity). The calculated (statistically averaged) mass resolved appearance curves and the kinetic energy distributions (KEDs) of the scattered C_n fragments revealed a precursor mediated, velocity correlated fragmentation event along the outgoing trajectory. Most of the larger fragments (n>5) are formed within a few picoseconds after leaving the surface, at vertical distances of 20-90 Å above the surface. The precursor time dependent structural transformations resembles formerly reported high temperature phase transition like behavior of fullerenes as observed in canonical ensemble simulations [2]. A complementary microcanonical ensemble simulation of the time evolution of an initially thermalized (superheated) C_{60} cage at 8500 K, over a few picosecond timescale, revealed a dynamics which seems to be similar to that of the impact generated precursor.

[1] Kaplan, A., Bekkerman, A., Tsipinyuk, B., and Kolodney, E. *Phys.Rev.B*, 79: 233405, 2009.
[2] Kim, S. G., Tomanek, D. *Phys.Rev.Lett*, 72:2418, 1994.