Current-induced Local Heating in Single Molecule Junctions

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Local heating is known to be an important factor in the design of conventional silicon-based microelectronics, so it is natural to ask how important this effect is in such electrode-molecule-electrode structures. Several theoretical calculations have found a finite increase in the temperature of the molecules as a result of inelastic scattering of electrons. However, measurement of current-induced local heating in a single molecule has not been carried out, due to the lack of a suitable experimental method. We have studied the current-induced local heating effects in single molecules covalently bound to two electrodes by measuring the force required to break the molecule-electrode bonds under various conditions. The breakdown process is thermally activated whichis used to extract the effective temperature of the molecular junction as a function of applied bias voltage. Wehave also performed first-principles calculations of both local heating and current-induced force effects, and the results are in good agreement with the experimental findings.
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