Simulation

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Why does a time-asymmetric behavior of macroscopic systems arise from a time-symmetric microscopic law? In 19th century, Boltzmann tried to verify the irreversible process of macroscopic systems using his elegant technique based on the kinetic equation and H-theorem. However, the problem on irreversibility remains unanswered because his approach drew many criticisms such as Loschmidt's reversibility paradox.

Recently, irreversibility has been investigated based on the chaos theory. In particular, a stability of N-body systems has been extensively studied by Molecular Dynamics (MD) methods. However, these MD methods can not avoid the numerical irreversibility due to round-off errors. For example, Loschmidt's reversibility paradox investigated by Orban and Bellemans. In their simulation, a time-reversal operation is realized by a velocity-inversion technique. That is, all velocities of the particles are reversed suddenly at a certain time in the middle of the equilibrium state. As a result, irreversibility appeared in the simulation, in other words, Boltzmann's H-function didn't return to the initial value after the time-reversal operation. (See 'Standard MD' in Fig.1. In Fig.1, time-reversal operations are applied at the timings designated by t_a and t_b.) To explain this result, they suggested that this irreversibility was due to round-off errors. Accordingly, it is still unclear whether the irreversibility of the system can be investigated properly, even if the stability has some relation to the irreversibility. This is because the numerical irreversibility may be dependent on the extent of round-off errors.

Therefore, to study the characteristic of this numerical irreversibility, we employ the 'bit-reversible algorithm' developed by Levesque and Verlet as a test bed. The bit-reversible algorithm (Bit MD) is completely time-reversible and is free from any round-off error and, therefore, any irreversibility can be detected definitely (see 'Bit MD' in Fig.1). This is because Bit MD employs Verlet's algorithm for time derivatives but, unlike the standard MD, employs a discrete coordinate space, instead of a continuous coordinate space. This complete time-reversibility suggests that, if a quantitatively-controlled noise is added to Bit MD, it may be possible to quantitatively investigate numerical irreversibility in the standard MD. Based on this idea, we investigate the irreversibility caused by the controlled noise added to Bit MD.

In this study, it is shown that even a negligibly-small deliberate noise can cause the irreversibility in N-body systems. It is found that the irreversibility is related not only to the extent of the instability of the system, but also to the 'quantity' of the controlled noise. From comparison with Bit MD added to the controlled noise of an appropriate *'quantity'*, the characteristic of the numerical irreversibility in the standard MD is revealed as shown in Fig.1.

35 - Investigation of the organic/organic interface in OLEDs by a Monte Carlo simulation

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General considerations for organic light emitting diodes (OLEDs) suggest that the carrier density is rather low in these devices. Along with the hopping charge transport characterizing the disordered organic materials of which these devices are made, it is clear that the Monte Carlo treatment is a normal way to investigate the functionality of OLEDs. A lot of work in the literature was devoted to theoretical and numerical study of the carrier conduction and injection at the metal/organic interface. However, very few papers address the problem of the organic/organic interface. This is in spite

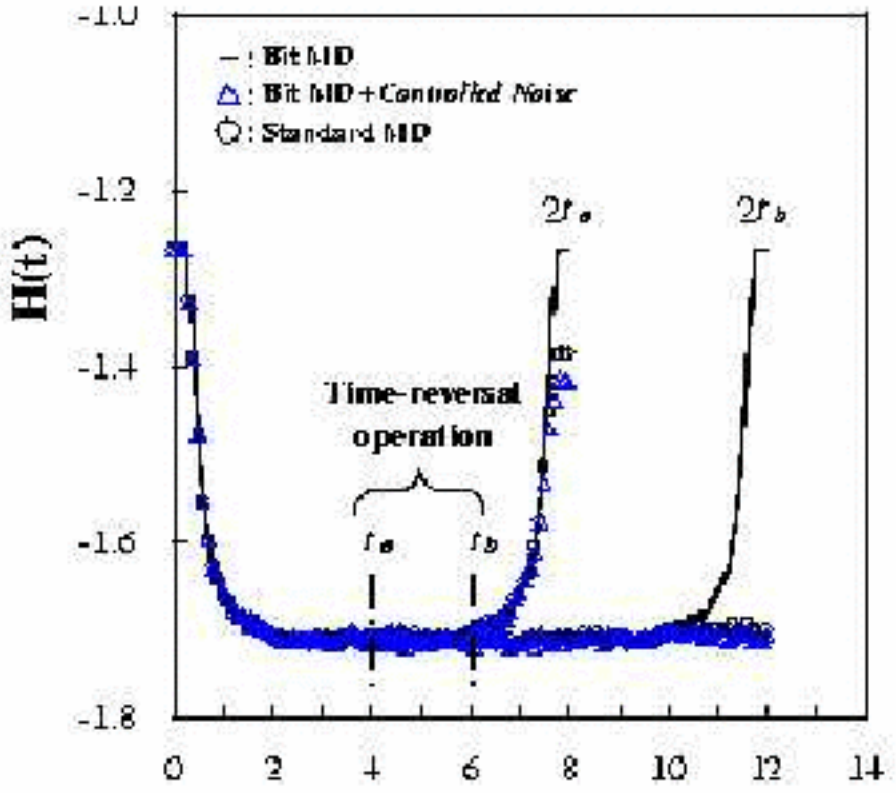

Figure 1: [34] Time evolution of H-function

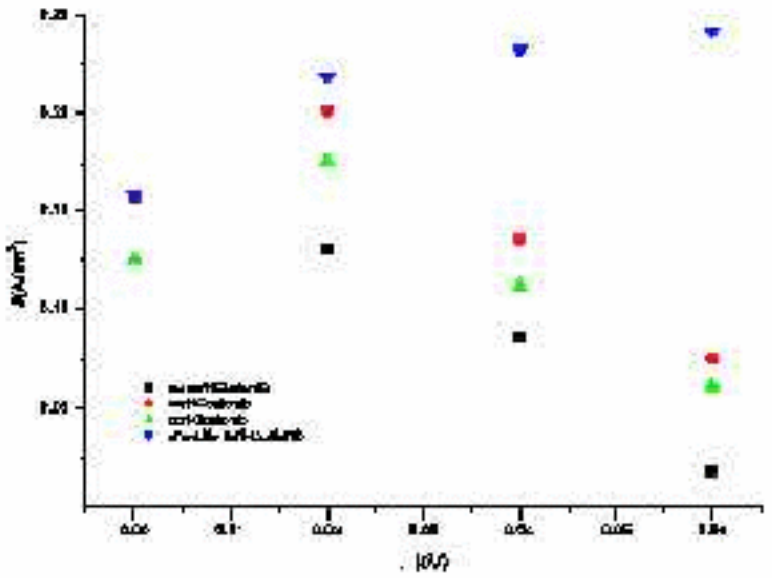

Figure 1: [35] Squares: non-correlated disorder; circles: correlated disorder; up-triangles: correlated disorder without Coulomb interactions; down-triangles: disorder on the second layer.

of the fact that the charge transport over organic/organic interfaces often dominates the device behavior and that most of the electron-hole recombination takes place there. Our simulations investigate the hopping transport across the organic/organic interface in a two-layer device. The model includes the Coulomb interactions among carriers and the effect of correlated Gaussian energetic disorder in the organic material. Hopping processes are modelled through the Miller-Abrahams hopping formula. The Monte Carlo procedure goes as follows: After computing the probabilities for each possible hop, the dwelling time for each electron and hole in the device is derived. The particle that hops first is the one with the shortest dwelling time. This many particle algorithm is suitable for programming on a parallel machine. The run time for reasonable values of the model parameters is of the order of several hours on eight 1.25GHz processors. Although the full model includes both electrons and holes and the recombination among them, in this communication we concentrate on the problem of the organic/organic interface in the monopolar (hole only) devices. The figure shows the evolution of the current of holes crossing the energetic barrier at the organic/organic interface as a function of disorder strength. The main observation is a decrease of the current with increasing disorder strength. However, when disorder exists only on one side of the interface (i.e. the second layer) the current increases with increasing disorder strength. It is only then that the widely used argument applies: that the disorder brings some energy levels of the second layer very close to the injecting level, thus reducing the effective energy barrier by an amount of σ^2/kT. However this argument does not apply to the three other cases studied here, where disorder is present on both sides of the interface. This is principally due to the fact that carriers tend to thermalize before jumping over the barrier. This is a consequence of the transversal hopping probability being much higher then the one perpendicular to the barrier leading the carriers to occupy the lower energy states. Thus the effective barrier is not very much altered beyond a certain value of disorder strength ($\sigma = 0.02eV$ in the figure).

36 - Density-functional investigation of alloyed metallic nanowires

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Density-functional band-structure calculations were carried out for two-shell metallic nanowires from Au and from AgAu and PdAu alloys. The investigated structures (cf. Fig. 1) contain 7, 9, and 18 atoms in the repeat unit along the wire direction, such that the central monoatomic chain is surrounded by 6 or 8 directly neighbouring atoms. All optimised structures are local minima of the formation energy, which are less stable than the unperturbed bulk phases, but more stable than the unreconstructed, planar Au(111) surface. Especially for low Ag or Pd contents the alloyed wires are even more stable than the respective pure Au, Ag, or Pd wires, i.e., the energy of mixing is negative and favours the alloying process. On the other hand, Au-centered wires with high Ag or Pd content exhibit a positive energy of mixing. Thus, alloying is unfavourable for wires with low Au contents, although the bulk alloy is stable. This deviation from the macroscopic behaviour is due to an internal stress balancing mechanism between tensile stress on the central chain and compressive stress on the outer shell. This balancing is possible for ultrathin, extended structures, but not in the isotropic bulk alloy.

The electron density difference between the two-shell wire and a superposition of the electron densities of the two shells from separate calculations was employed to analyse the inter-