Tang *et al.* Reply: The central issue raised by Ding *et al.* [1] is whether molecular dynamics (MD) simulations can capture the main physics underlying the superplastic deformation of carbon nanotubes (CNTs) at high temperatures [2]. They have no quarrel with any technical aspects of our MD calculations; instead, they raise the issue on the higher simulation strain rate compared to that employed in the recent experiment [2] and offer an alternative interpretation to describe the observed superelongation of CNTs. Here we point out that (1) the large deformation of CNTs at high temperatures involves complex dynamics that hold the key to understanding this intriguing phenomenon and (2) MD simulations have considerable advantages in describing the dynamic processes and the atomistic mechanism for defect generation, distribution, and propagation on the tube wall at large strains and high temperatures. Despite constraints imposed by computing capacity (e.g., the use of fast strain rate), MD calculations such as those reported in our work represent the current state of the art in large-scale simulations of physical processes and are generally recognized for their value and usefulness in materials research.

The main idea of the proposed alternative analysis is based on a previous work [3] that suggests that the superelongation of CNTs can be described by the nucleation of a few 5–7 defects and their subsequent propagation along an ideal helical pathway. This kinetic analysis is based on static energetic calculations on optimized crystal structures without considering the influence of temperature on the lattice parameters. However, at high temperatures significant lattice fluctuations occur and deviations from their equilibrium states can be very strong [4]. A fully dynamic approach is required to properly account for the activation and distribution of a rich variety of defects other than the lowest-energy configuration, which are expected to exist on tube walls as governed by statistical physics principles. The statistical nature of the problem also affects the propagation of the defects. In our MD simulations [5,6] temperature effect is explicitly incorporated. Our results reveal the nucleation of a large amount of topological defects near the elastic limit and their subsequent random motion in the dynamical process. This is consistent with recent high-resolution atomic imaging experiments that show random movement of defects on the tube wall [7].

A close examination of experimental results also suggests there is a significant (over 75%) mass loss during the elongation process [2]. These large number of mass-loss sites and the associated defects are likely to be randomly distributed. In addition, it is noticed that the single-wall CNT (SWCNT) sample was obtained by an electrical breakdown of a multiwall CNT (MWCNT). An early experiment using a similar approach shows that the electrical breakdown is induced by Joule heating to all layers of the MWCNT [8]. It is therefore natural to expect that a large amount of defects have already been introduced into the remaining layer of the sample during the preparation process. Additional topological defects can be introduced by the follow-up heat treatment [7] and by the irradiation effect inside TEM. Furthermore, the experiment shows that the measured electric current passing through the SWCNT decreases continuously during the stretching process [2], which implies a continuous increase of the defect concentration in the tube wall.

Our MD simulations were conducted below the sublimation temperatures and, therefore, do not address the issue of atomic mass loss. Computational limitations also require the use of strain rates much higher than those used in experiments. Despite these constraints, MD simulations offer an appealing approach to complement the kinetic analysis and the associated energetic and empirical modeling calculations. In particular, MD allows one to explore the complex dynamics important at high temperatures and the underlying atomistic mechanisms. The strain rate effect remains an open issue that deserves further investigation. A recent experiment shows that the dynamic process of reaction front can occur at a speed of 13 m/s [9], which is faster than our simulated strain rate. This result underscores the need to explore phenomena over a large range of strain rate, especially fast processes that can be handled by MD very well.

In conclusion, MD simulations have advantages in describing the dynamics underlying the CNT deformation processes. Our calculations revealed the important role of widely distributed topological defects on the superplastic deformation of SWCNTs at high temperatures [5,6]. The effects of atomic sublimation and slower strain rate on CNT deformation may introduce new physics and deserve further exploration.

Chun Tang,[1,2] Wanlin Guo,[2] and Changfeng Chen[1]
[1]Department of Physics
and High Pressure Science and Engineering Center
University of Nevada
Las Vegas, Nevada 89154, USA
[2]Institute of Nano Science
Nanjing University of Aeronautics and Astronautics
Nanjing 210016, China

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