



# Monatomic metal nanowires: Rupture kinetics and mean lifetime



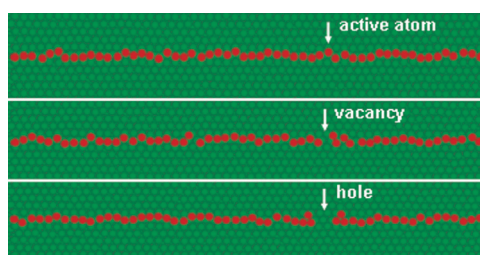
Michail Michailov\*, Dimo Kashchiev

Institute of Physical Chemistry, Bulgarian Academy of Sciences, ul. Acad. G. Bonchev 11, Sofia 1113, Bulgaria

## HIGHLIGHTS

- Spontaneous rupture of monatomic metal nanowire on (111) crystal face occurs in three steps.
- Steps 1 is formation of active atoms, step 2 is appearance of atomic vacancies, step 3 is birth of hole.
- The first few vacancies and holes in the nanowire appear randomly according to a Poisson process.

## GRAPHICAL ABSTRACT



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## ABSTRACT

We present a model for the kinetics of spontaneous (unforced) rupture of monatomically thick metal nanowire on atomically smooth crystal face. The nanowire breaks down spontaneously solely because of the thermal motion of the atoms in it and the underlying crystal. Our model describes the nanowire rupture as a three-step process involving (i) appearance of atoms active in vacating their positions, (ii) generation of atomic vacancies, and (iii) formation of holes (vacancy dimers) in the nanowire. The model is based on Monte Carlo simulation results for the temporal evolution of initially straight monatomic chain of Cu atoms on Cu(111) crystal face. The simulation provides data for the time dependence of the number  $N_v$  of vacancies and the number  $N_h$  of holes in the nanowire, as well as for the probabilities  $P_v$  and  $P_h$  to form, respectively, at least one vacancy and at least one hole until time  $t$ . We describe the nanowire rupture kinetics by using rate equations and obtain expressions for the nanowire mean lifetime and the  $N_v(t)$ ,  $N_h(t)$ ,  $P_v(t)$ , and  $P_h(t)$  dependences. These expressions are found to conform well to the simulation data, which implies a Poissonian random appearance of the first few vacancies and holes in the nanowire.

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## 1. Introduction

Among the various nanoscale systems in materials science, the one- or several-atom thick nanowires hold special attention because of their great scientific and technological importance. The reduced dimensionality and size of these thinnest nanowires excite remarkable academic curiosity in relation to their structure, stability, and quantum properties (e.g. [1–16]). The thinnest nanowires promise to have intriguing applications in

nanoelectronics, catalysis, optics, and sensor technology. Prepared by scanning tunneling microscopy (STM) tip-based methods or break-junction techniques, or formed on vicinal and atomically smooth crystal surfaces, the monatomic metal nanowires are regarded as the ultimate quantum conductors [17]. These ultrathin atomic chains offer the possibility to tune the electron transport in them in a way that leads to ballistic conduction, a situation when the electrons propagate freely without scattering. As this type of conduction and other exotic features of the nanowires are strongly dependent on the nanowire size and shape, detailed knowledge of the nanowire structure and stability is indispensable.

Addressing a cutting-edge issue in materials science, the theoretical and experimental studies on the thinnest nanowires have

\* Corresponding author.

E-mail address: [mike@ipc.bas.bg](mailto:mike@ipc.bas.bg) (M. Michailov).

hitherto been mainly focused on the question of how to create such nanowires (e.g. [1,2,6,13,18–26]). Considerably less attention has been paid to the nanowire stability with respect to rupture. Besides, in almost all papers considering this problem, only forced nanowire rupture has been investigated (e.g. [1,6,8,14,16–18,20–22,26–34]). This kind of rupture occurs when the nanowire is under the action of external factors such as stretching [8,32], alloying [34] or applied voltage [27,30]. These factors affect the nanowire breakdown by changing such parameters as the distance between the atoms in the nanowire, the strength of the bonds between these atoms, and the nanowire temperature.

In contrast with the investigations on forced nanowire rupture, the present study is concerned with the question of how a nanowire breaks down spontaneously, i.e. as a result solely of the thermal motion of the atoms in it. In a nanoscale system, this motion may deviate substantially from that on the macroscale, which in turn may lead to considerable changes in the physical behavior of the system. Examples in this respect are the unusual thermal diffusivity and phonon energy inversion of a graphene nanoribbon which result from the dynamic response of the nanoribbon to thermal excitation [35,36].

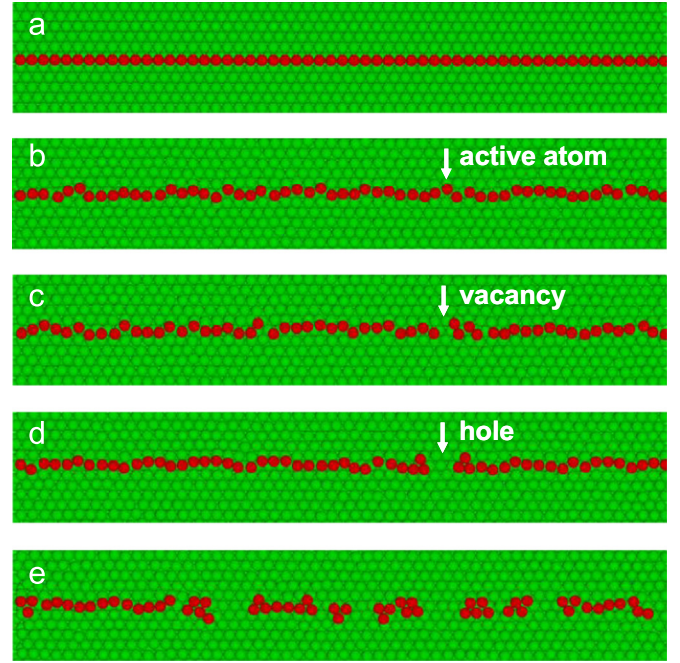
But why should a monatomic nanowire, either free standing or on a substrate, break down by itself when it is not affected by external factors and does not lose its atoms by evaporation or dissolution? The fundamental physical reason is that its free energy is appreciably higher than that corresponding to the equilibrium shape of the cluster constituted of the same number of atoms. The nanowire atoms are thus bound to rearrange themselves into equilibrium-shape cluster, because this new atomic configuration ensures minimal free energy. To follow any of the various possible kinetic pathways to this configuration, the nanowire has first to rupture into two or more pieces when its two ends are pinned. Being shorter nanowires with already mobile ends, the nanowire fragments have the possibility to transform their shape towards the equilibrium one, and if capable of moving, to merge into a single, equilibrium-shape cluster. Besides, under otherwise equal conditions, a free-standing nanowire may be expected to break down much more rapidly than a nanowire on a substrate, because it cannot experience the possible stabilizing effect of the nanowire/substrate interaction. This effect can be particularly strong for monatomic nanowires formed along atomic channels on the substrate (the (110) crystal face is a good example of such a substrate [25]).

Based on our recent work [37] on the kinetics of thermal rupture of a chain of single Cu atoms on Cu(111) substrate, here we present a general scenario for spontaneous breakdown of monatomically thick metal nanowire on atomically smooth crystal face. Our objective is to reveal the time evolution of the nanowire morphology at the atomic scale and, thereby, to identify the mechanism of spontaneous nanowire rupture. Also, we employ rate equations to describe the respective rupture kinetics and derive expressions for a number of physically important and experimentally accessible quantities such as the probability for nanowire rupture and the nanowire mean lifetime.

## 2. Methods

### 2.1. Physical model

In the present simulation experiment we consider a monatomically thick metal nanowire (a chain of single metal atoms) on an atomically smooth crystal face of the same metal (Fig. 1). As the nanowire is not affected by external factors, its stability with respect to rupture is controlled solely by the atomic thermal motion. Initially (Fig. 1(a)), the system is a perfectly ordered fcc Cu crystal



**Fig. 1.** Successive snapshots of monatomic nanowire at (a)  $t = 0$ , (b)  $t = 900$  MCS, (c)  $t = 1300$  MCS, (d)  $t = 4200$  MCS, and (e)  $t = 9900$  MCS. The red and green spheres represent nanowire and substrate atoms, respectively, and the arrows indicate an active atom (panel (b)), the first vacancy (panel (c)), and the first hole (panel (d)) in the nanowire. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

substrate with an ideally straight chain of Cu atoms on the (111) face of the substrate. The nanowire is constituted of 57 Cu atoms, and the substrate is a rectangular parallelepiped with length and width of 57 and 33 Cu atoms, respectively, and with thickness of 5 Cu monolayers subjected (along with the nanowire) to periodic boundary conditions.

### 2.2. Computational model

In the computations, we employed a many-body tight-binding (second-moment approximation of the electron density of states) potential between the interacting metal atoms [38]. This semi-empirical potential has already been applied to simulate metal nanowires at the atomic scale (e.g. [7,28,29,33,37]). Its wide application also to transition metals and intermetallic alloys is due to its ability to faithfully reproduce real physical properties of bulk metals and their surfaces with steps, kinks, point defects, dislocations, vacancies, and grain boundaries [38–40].

The energy  $E_i$  of atom  $i$  in the system is a sum of repulsive ( $E_i^r$ ) and attractive ( $E_i^b$ ) interaction terms:  $E_i = E_i^r + E_i^b$ . These terms are given by the expressions [38]

$$E_i^r = A \sum_j \exp \left[ -p \left( \frac{r_{ij}}{r_0} - 1 \right) \right] \quad (1)$$

$$E_i^b = -\xi \left\{ \sum_j \exp \left[ -2q \left( \frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{\frac{1}{2}} \quad (2)$$

where  $r_{ij}$  is the distance between atoms  $i$  and  $j$ , and  $r_0$  is the nearest-neighbor distance in the metal lattice. The parameters  $A$ ,  $p$ ,  $\xi$  and  $q$  have values obtained by fitting to experimental data for the cohesive energy, lattice parameters and independent elastic constants of the metal system studied. For our monatomic homoepitaxial Cu/Cu(111) nanowire we used the  $A$ ,  $p$ ,  $\xi$  and  $q$

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