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Thermal stability and spontaneous breakdown of free-standing metal nanowires



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ABSTRACT

We present a model for vacancy-mediated spontaneous breakdown of free-standing monatomic nanowire based on exclusively random, thermally activated motion of atoms. The model suggests a new twostep vacancy-mediated mechanism for nanowire rupture compared to the more complex three-step hole-mediated mechanism driving the disintegration of nanowire on crystalline surface. It also demonstrates that a free-standing nanowire breaks down much more rapidly than a nanowire on a substrate, because it cannot experience the stabilizing effect of the nanowire/substrate interactions. The rupture mechanism includes single atomic vacancy generation, preceded by appearance of weakly bonded active atoms. The analysis of the simulation data indicates that the active atoms act as a precursor of vacancy formation. These two successive events in the temporal evolution of the nanowire morphology bring the free-standing nanowire into irreversible unstable state, leading to its total disintegration.

The present study also manifests an unexpected substantial increase of the nanowire lifetime with diminishing the strength of the atomic interactions between the nanowire atoms. The simulation data reveal three energy regions where a large oscillatory variation of nanowire lifetime is realized. The first region of strong atomic interactions is characterized by tight nanowire rigidity and short lifetime. The next, second region in the consecutive step-down of the attractive interatomic force is characterized by generation of wave-shaped morphology of the atomic chain, enhanced flexibility and dramatic increase of nanowire lifetime. In the last, third region, further weakening of the interactions returns the nanowire again to unstable, short-lifetime state. The observed phenomenon is considered as a "stick-like" to "polymer-like" transition in the nanowire atomic structure as a result of interaction energy variation. The enhanced flexibility reduces the nanowire free energy since it favors and facilitates the rate of entropy propagation in the atomic chain structure. The observed phenomenon opens a way for a new type atomic scale control on the thermal stability of both free-standing nanowire and nanowire on crystalline substrate. The present study also extends the validity of the three-step breakdown mechanism of nanowire on crystalline substrate to the specific case of thermally activated free-standing nanowire rupture not affected by any external forces.

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1. Introduction

Metal atomic nanowires hold special attention in contemporary materials science because of their great scientific and technological importance. These low-dimensional linear structures excite also remarkable academic curiosity in relation to their structure, stability, and quantum properties [1–12]. The exotic physical features of metal nanowires also provide a challenging background for a large number of applications in nanoelectronics,

* Corresponding author. E-mail address: mike@ipc.bas.bg (M. Michailov). optics and catalysis. Being a cutting-edge problem in the nanoscale physics, the theoretical and experimental studies on the thinnest nanowires have hitherto been mainly focused on the question of how to create nanowires [1-3,9]. Considerably less attention has been paid to the nanowire stability, rupture and complete disintegration [11,12]. That is why, the present study deals with the problem of how a single nanowire breaks down spontaneously, exclusively as a result of the thermal motion of the atoms in it.

Recently, a new physical model for spontaneous, hole-mediated breakdown of monatomic metal nanowires on crystal surfaces has been suggested [12]. The physical scenario of the breakdown process implies three consecutive steps of nanowire rupture including: (i) formation of active atoms, (ii) generation of single atomic

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vacancy and (iii) evolution of the single vacancy into a two-vacancy cluster (called hole). In all these steps involved into the nanowire rupture, illustrated in Fig. 1, the influence of the substrate is significant. The substrate affects the nanowire stability in different ways. It can stabilize or, in contrast, facilitate the nanowire breakdown depending on its anisotropy, softness of the surface potential, lattice misfit between substrate and nanowire, etc. Special attention has to be paid to the role of incommensurability with the crystalline surface. In some cases, the lattice mismatch could be crucial for the nanowire breakdown and its total disintegration. The contribution of these simultaneously acting, competing effects is controlled by the substrate/nanowire interface energy minimization. Since a large number of experiments deal with the nanowire features on a substrate, in the present study we discuss the thermal properties of a free-standing monatomic nanowire in vacuum where the influence of the substrate is entirely avoided. In this way, we assess more clearly the impact of the atomic interaction potential on the nanowire stability and reveal the nanowire breakdown scenario in the absence of external field. Hence, we focus our study on the following questions: (i) Could the model of vacancy- and holemediated nanowire rupture, valid for nanowire on surface, be extended to a free-standing nanowire? (ii) What is the influence of the strength of the interactions between the nanowire atoms on the nanowire morphology, atomic structure and stability? (iii) How does the nanowire flexibility affect the nanowire thermal stability? The answers to these questions could contribute to a better understanding of the fundamental mechanism of monatomic



Fig. 1. Hole-mediated breakdown of a nanowire on crystalline surface. The time evolution reveals multistep rupture mechanism leading to total nanowire disintegration. (a) Initial configuration. (b) Formation of active sites (precursors) at 200 MCS. (c) Generation of single vacancy at 500 MCS. (d) Generation of hole (double vacancy) at 2800 MCS. (e) Formation of atomic clusters at 9900 MCS (after Michailov and Kashchiev [12]).

nanowire breakdown and its complete disintegration which is a matter of great importance in contemporary interface materials science [1–7].

2. Physical and computational models

The physical model in the present study is designed to reveal the time evolution of free-standing monatomic Cu chain in vacuum at constant temperature *T*. The atoms which are exposed to thermal fluctuations only are bound via interacting potential. The computational model is grounded on classical canonical Monte Carlo (MC) sampling with many-body Tight Binding Second Moment approximation (TB SMA) potential between atoms [13–16]. In this approach, the total interaction energy E_i of atom *i* in the system is expressed by

$$E_i = E_i^r + E_i^b,\tag{1}$$

with E_i^r and E_i^b being, respectively, the repulsive and attractive energy terms. Explicitly, E_i is given by [13]

$$E_{i} = \sum_{j, r_{ij} < r_{c}} A \exp\left[-p\left(\frac{r_{ij}}{r_{0}}-1\right)\right] - \sqrt{\sum_{j, r_{ij} < r_{c}} \xi^{2}} \exp\left[-2q\left(\frac{r_{ij}}{r_{0}}-1\right)\right]$$
(2)

where r_{ii} is the distance between atoms *i* and *j*, r_0 is the nearestneighbor atomic distance of the corresponding pure metal, A and p are energy- and compressibility-related free parameters, and r_c is the cutoff distance for the interaction. The first term in Eq. (2) is a Born-Meyer type ion-ion repulsion and the second term is the bond energy term, obtained in the form of the second-moment approximation of the electron density of states [13]. In Eq. (2), ξ is an effective hopping integral and *q*describes its dependence on the relative interatomic distance. In general, the expression for E_i^b , can be considered as a sum over the local electronic charge density induced at site *i* from the atoms at site *j*. Hence, ξ is expected to be sensitive to the number of surrounding atoms in all space directions. The energy calculation is performed over all atoms within a sphere having radius 3 times the Cu-Cu nearest-neighbor distance in the bulk crystal. The values of the hoping integral ξ and all related parameters *A*,*p*, and *q* in Eq. (2) are taken from [13,15]. The statistical distribution in our model is canonical, i.e., ensemble with constant number of particles at fixed temperature and volume [16]. In equilibrium, the system energy reaches its minimum and fluctuates around a constant value. Full lattice dynamics of all nanowire atoms ensures complete relaxation of the system. All simulations are grounded on three-dimensional continuous space model, i.e., nanowire atoms are able to change their positions in all space directions with a step of 0.05 units of the lattice constant. The initial nanowire configuration is a perfectly ordered linear monatomic chain with periodic boundary conditions along the chain axis. All simulation data are averaged over 50 runs with single nanowire for each temperature and each value of the attractive term in the interaction potential in Eq. (2). The nanowire length is 76 atoms. The variation of the nanowire morphology and its atomic structure are monitored by a series of successive snapshots taken at every 10 Monte Carlo Steps (MCS). In all simulations, the nanowire follows the classical thermodynamic pathway towards equilibrium of an ensemble of atoms by minimization of the system energy via clustering. Complete simulation details are described elsewhere [12,15].

3. Results and discussion

The first part in the present study is devoted to the breakdown mechanism of free-standing nanowire and evaluation of its mean lifetime at a fixed temperature. Let us point out that our analysis is based on a physical scenario involving three-step hole-mediated mechanism for a rupture of nanowire on a crystal substrate [12]. The simulation experiment presented here reveals the time evolution morphology of initially perfectly ordered, standing freely in vacuum, atomic chain. It also gives evidence for the moment of appearance of the first single atomic vacancy, as well as for the ensuing total nanowire disintegration. As seen in Fig. 2a, the free-standing monatomic nanowire in its initial state consists of regularly ordered atoms, all being passive with respect to their ability to form a vacancy, because they have equal probability to leave the atomic chain. This state is followed by generation of active atoms which are shifted from their initial positions at a distance larger than half atomic diameter, Fig. 2b. These atoms are weakly bound to their neighbors and therefore they could give birth of single atomic vacancies appearing randomly in both space and time, Fig. 2c. Later, these vacancies transform into vacancy holes, Fig. 2d, subsequently leading to non-recoverable rupture and total nanowire disintegration, Fig. 2e. The simulation data analysis shows that because of the absence of substrate (a substrate potential would stabilize the nanowire), the free-standing nanowire breaks down at considerably earlier moment of its temporal evolution. Moreover, due to increased thermal fluctuations of the weakly bound atoms (they lack bonds with the substrate), nanowire breakdown occurs exclusively at low temperatures, below 50 K. Simulations at T = 300 K demonstrate instantaneous disintegration in the range of about 10 MCS. The time evolution of the atomic morphology is shown in Fig. 2. At 200 MCS, formation of single atomic vacancies is evident. They grow to larger vacancy holes at a later stage of 400 MCS of the nanowire evolution. At 1200 MCS, the rupture-generated small atomic chains tend to form spherical clusters, thus reducing their free energy. Let us remind here that periodic boundary conditions are imposed on our free-standing nanowire (comprised of 76 atoms) and therefore it behaves as an infinite linear atomic chain. Hence, the formation of atomic clusters is possible only for the nanowire parts of finite number of atoms (finite length atomic chains) created after the nanowire breakdown, i.e., after the random appearance of atomic vacancies and atomic holes, Fig. 2c-e. It is important to note that the clusters tend to agglomerate and at sufficiently long evolution time they all form only one large cluster. This trend is clearly seen in Fig. 2d and e where the third and fourth clusters (from left to right in Fig. 2d) at a later time form only one, single cluster (third cluster in Fig. 2e). This scenario is fully in line with the classical Gibbs thermodynamics and follows the natural system pathway towards equilibrium by minimization of the free energy of the ensemble of atoms that belong to the nanowire. All these processes can be classified as consecutive steps of events leading to formation of a single atomic vacancies, holes and complete disintegration of the atomic chain at a later stage. This classification includes the following transitions:

$$P \xrightarrow{\omega_{pa}} A \xrightarrow{\omega_{av}} V \xrightarrow{\omega_{vh}} H$$
(3)

Here P, A, V and H stand for passive atom, active atom, vacancy and hole respectively, and ω_{pa} , ω_{av} , and ω_{vh} are the frequencies of P–A, A–V and V–H transitions, respectively.

Detailed analysis of the simulation data reveals that once an active atom, single atomic vacancy or hole is created, its disappearance by thermally activated and randomly moving neighboring atoms is highly unlikely at T < 50 K. That is why, in the above reaction scheme, we can neglect the contribution of all reverse transitions A–P, V–A and H–V. This result is in contrast with the thermal behavior of nanowire on substrate, where the recovering of active atoms and single vacancies takes place with a considerable probability because of the impact of the substrate potential.

The observed thermal behavior of the free-standing nanowire implies a similar breakdown mechanism as that of the nanowire on substrate. At the same time, two basic differences which do not change the physical picture of the observed nanowire rupture have to be pointed out. The first relates to the absence of recovering mechanism after the generation of single atomic vacancy. The second and most important difference is that single vacancy formation already causes complete nanowire breakdown. Therefore, the generation of hole is not required for the total nanowire disintegration, as it is in the case of substrate-supported nanowire. Accounting for these differences, after the necessary simplifications, we can use the available results for nanowire on substrate [12]. Hence, for the average number N_{ν} of vacancies as a function of time *t*, we have

$$N_{\nu}(t) = (1/2)\omega_{pa}\omega_{a\nu}N_0t^2 \tag{4}$$

where N_0 is the number of atoms in the nanowire. Let us point that the above transition frequencies are time- and space-independent, but are strongly influenced by the temperature. The initial stage of nanowire rupture according to the multistep model schematized by Eq. (3) is confirmed by fitting the simulation $N_v(t)$ data by Eq. (4) (see Fig. 3).

It is important to note that the simulation data give also evidence for the role of the active atoms as precursors of the nanowire breakdown. In the initial stage of the nanowire time evolution, we observe a characteristic delay in vacancy formation which reveals clear necessity for generation of a certain number of active atoms before the actual birth of a single vacancy. If the rupture process is precursor-free (or in our case "active atomfree"), the increase in the number of vacancies (Fig. 3) would begin without any delay. The rupture mechanism of free-standing nanowire is thus characterized by a certain time lag for generation of active atoms preceding and causing the birth of vacancies. Therefore, accounting for all particularities presented here, the free-standing monatomic nanowire breakdown has to be considered as occurring by a two-step vacancy-mediated mechanism compared to the three-step hole-mediated mechanism for a nanowire on a crystalline surface.

The second part of our study deals with the impact of the atomic interactions on the nanowire stability. Being free-standing and therefore not affected by external field, the nanowire tries to keep its own geometry as a linear atomic chain. Therefore, at very



Fig. 2. Free-standing monatomic Cu nanowire at temperature 10 K. Snapshots at different times indicate: (a) initial configuration; (b) generation of active atoms; (c) formation of vacancies; (d) formation of holes; (e) total nanowire disintegration. At 4000 MCS, the agglomeration of atomic clusters already formed at 1200 MCS is seen.

low temperature, at which the thermal fluctuations are notably weak, the atomic chain behaves like a "stick". Our observations indicate that during the nanowire time evolution, all thermally activated atoms shift from their positions preferentially in direction following the initial straight line connecting the nanowire. Let us remind that both repulsive and attractive interactions act exclusively along this line due to the linear atomic arrangement. This is clearly seen in Fig. 2b and c, where both P–A and A–V transitions take place by displacements solely along the initial nanowire line. This behavior is entirely different from that of a nanowire on crystalline surface where the atomic shifts are tightly influenced by the strength and anisotropy of the surface potential (see Fig. 1).

Our simulations at two temperatures T=10 and 50 K reveal that a decrease of the interaction energy by variation of the attraction term in Eq. (3) causes significant increase of the nanowire lifetime. This effect is manifested clearly in Fig. 4 where the nanowire morphology is seen at four different values of the attractive term in the interaction potential. The evolution of all nanowires is shown for a fixed period of time and all snapshots are taken at the same moment t=6000 MCS.

The first snapshot, Fig. 4a, relates to nanowire with attraction energy identical to that for the bulk Cu crystal, $\xi = 1.224$ eV. As it has to be expected, the complete, irreversible disintegration of the chain leads to formation of small atomic clusters. Before its rupture, this nanowire has a high rigidity and a stable "stick-like" morphology. Decreasing the attractive atomic interaction to $\xi = 0.924$ eV increases dramatically the nanowire lifetime, Fig. 4b. Further diminishing of ξ to 0.724 eV enhances the nanowire stability and produces light wave-shaped modulation of the linear

atomic arrangement, Fig. 4c. At this interacting potential, the nanowire has an increased flexibility and manifests "polymer-like" behavior. Continuous decrease of ξ keeps the nanowire stable and hinders the vacancy formation up to ξ =0.224 eV when the atomic chain starts again to generate vacancies and becomes unstable. The observed unexpected phenomenon of enhanced nanowire stability after decrease of the force acting between its atoms is clearly seen also in Fig. 5.

It is essential to point out that the simulation of the nanowire temporal evolution is limited to time t=30,000 MCS and therefore the nanowire lifetime relates exclusively to this period. As seen in Fig. 5, at T=10 K in the energy range 0.4–0.9 eV the lifetime exceeds 26,000 MCS which is two orders of magnitude higher than the lifetime at high and low attractive energies outside this region at the same temperature.

The analysis of the simulation data reveals distinctly three regions in the energy dependence of the nanowire lifetime. The first region is limited to 1.224-0.9 eV where the nanowire follows the two-step vacancy-mediated mechanism of rupture, already discussed in the first part of the present study, and has a relatively short average lifetime of 250 MCS at T = 10 K. The third region characterized by low, less than 0.3 eV, attractive energies reveals a lifetime similar to that in the first region. The main difference here is the nanowire atomic morphology. This morphology suggests that as a result of very week mutual attraction, the atoms can shift easily also in other directions and may generate active atoms different from that of the free-standing nanowire at low temperature. These active atoms are positioned similarly to these in the case of nanowire on substrate, Fig. 4d. Evidently, most exciting is the second region defined for energies 0.3-0.9 eV where the nanowire lifetime dramatically increases. This energy range is characterized with peculiar morphology of the atomic chain. The decreased



Fig. 3. Time dependence of the average number of vacancies, N_{ν} , at T=10 K (open circles) and T=50 K (solid circles). The simulation data are fitted (solid lines) by Eq. (4).



Fig. 5. Average time for generation of the first atomic vacancy vs. attractive energy between the nanowire atoms at T=10 K (open circles) and T=50 K (solid circles). Significant increase of the nanowire lifetime is seen in the energy region 0.4–0.9 eV.





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interaction enables the generation of thermally activated waveshaped structure, which strongly affects the nanowire stability. The lengthened nanowire lifetime in this region originates not only from the reduced amplitude of the thermal fluctuations at low temperature (T=10 K) which are not able to overcome the interatomic binding energy. The weak attractive forces between atoms do not favor rupture of the atomic chain and formation of atomic clusters, because, being weakly bound, the atoms of the chain form a structure with decreased rigidity. Hence, the subtle competition between increased chain flexibility and confined thermally activated atomic shifts produces a relatively stable wave-shaped nanowire. Let us point out also that precise analysis of the observed phenomena requires the increased entropy contribution to be accounted for, too. This evaluation is a problem of separate study. The increased nanowire flexibility facilitates the entropy propagation during the nanowire temporal evolution towards equilibrium and increases the rate of entropy generation in the system. Therefore, we can consider the nanowire morphology variation from the first to the second interaction-energy region as a "rigidity-flexibility" state transition or a "stick-like" to "polymer-like" switch. The analysis of our simulation data for both the mean nanowire lifetime and the nanowire morphology clearly demonstrates that weakly bonded nanowires are more stable at low temperature, compared to nanowires with strongly interacting atoms at the same temperature.

To clarify the observed increased nanowire flexibility, we have also analyzed the variation of the inflection-point position in the nanowire interacting potential as a function of the value of the decreasing attractive interaction ξ in Eq. (2). This position influences the ability of an atom to leave the chain structure and to produce a vacancy (see Fig. 6). Being more or less displaced from the minimum of the interacting potential, it also controls the equilibrium mean distance between atoms. The decrease of the attractive force (attractive branch of interactions in Fig. 6) leads to a shift of the inflexion point towards a larger distance between the atoms. Hence, this shift causes enhanced flexibility and easier relaxation of the atomic chain. Therefore, the "stick-like" to "polymer-like" nanowire transition, which substantially influences the nanowire lifetime, is a complex phenomenon originating from the variation of the position of the inflection point in the interacting potential and the entropy contribution.

The above analysis suggests a new mechanism for control of the nanowire lifetime. Hence, besides the obvious way of lifetime



Fig. 6. Tight-binding potential used in our simulations at different attractive energies. The arrows indicate the position of the inflection point for two different values of ξ . Inset: inflection-point position as a function of ξ .

manipulation via simple temperature variation, a different approach could be applied to control the nanowire disintegration or stabilization. For easier breakdown we have to increase the nanowire rigidity or, in contrast, for stabilization we have to increase the nanowire flexibility. Therefore, given two different free-standing nanowires, the one with relatively weakly bound atoms is expected to have a higher stability and, accordingly, a longer mean lifetime.

4. Conclusion

The present study provides insight into the breakdown mechanism of free-standing monatomic metal nanowires. Being exposed exclusively to thermally activated, random displacements, the nanowire atoms generate single atomic vacancies which cannot be recovered and cause a total disintegration of the linear atomic structure. The vacancy formation is preceded by appearance of weakly bound active atoms playing the role of vacancy precursors. Analyzing these successive events in the temporal evolution of the nanowire morphology, we observe a new twostep rupture mechanism for free-standing nanowire breakdown. This mechanism is a particular case of the more complex, threestep rupture scenario of substrate-supported nanowires. The simplification in the case of free-standing nanowire is a result of the missing impact of the substrate surface potential which stabilizes the nanowire by enabling it to repair some of the already generated atomic vacancies. The two-step breakdown scenario makes it possible the results already obtained for the rupture kinetics of nanowires on substrates to be applied to free-standing nanowires. In this way, the present study extends the validity of the three-step nanowire breakdown mechanism [12].

The simulation data also reveal an unexpected nanowire lifetime behavior during the variation of the force acting between the nanowire atoms. In a specific energy region, the decrease of the attractive term in the atomic interactions leads to significant nanowire stabilization, Figs. 4 and 5. The nanowire lifetime is enhanced more than two orders of magnitude. Our detailed analysis reveals that this variation is due to a shift of the interaction potential inflection point, Fig. 6. The displacement toward larger distance from the potential minimum makes it possible the atom thermal motion not to be tightly confined along the straight line of the ideal atomic arrangement. The thermal fluctuations become more pronounced in other space directions. The decrease of interatomic force also renders the nanowire less rigid and thus, by increasing its flexibility, facilitates and promotes the entropy propagation in the atomic chain. This effect of increased nanowire flexibility is confirmed in our simulation by the appearance of standing waves illustrated in Fig. 4b and c. The observed phenomenon could be considered as a "stick-like" to "polymer-like" transition in the monatomic chain which has a strong impact on the nanowire lifetime and thermal stability. It is important to point out that the stabilization effect resulting from enhanced nanowire flexibility is expected to be valid in the case of nanowire on a substrate, too. Experimental research in this direction could significantly contribute to a better understanding of the methods for atomic-scale control of the nanowire lifetime and rupture kinetics.

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References

- [1] N. Agrait, A.L. Yeyati, J.M. van Ruitenbeek, Phys. Rep. 377 (2003) 81.
- [2] A.I. Yanson, G. Rubio-Bollinger, H.E. van den Brom, N. Agrait, J.M. van Ruitenbeek, Nature (London) 395 (1998) 783.
- [3] M. Kiguchi, T. Konishi, K. Murakoshi, Phys. Rev. B 73 (2006) 125406.
- [4] U. Landman, R.N. Barnett, A.G. Scherbakov, P. Avouris, Phys. Rev. Lett. 85 (2000) 1958.
- [5] E. Tosatti, S. Prestipino, S. Kostlmeier, A. Dal Corso, F.D. Di Tolla, Science 291 (2001) 288.
- [6] I.K. Robinson, P.A. Bennett, F.J. Himpsel, Phys. Rev. Lett. 88 (2002) 096104.
 [7] N. Agrait, C. Untiedt, G. Rubio-Bollinger, S. Vieira, Phys. Rev. Lett. 88 (2002) 216803.
- [8] S. Pelaez, C. Guerrero, R. Paredes, P.A. Serena, P. Garcia-Mochales, in: N. Lupu (Ed.), Electrodeposited Nanowires and Their Applications, In Tech, Rijeka, 2010, p. 35.
- [9] H. Onishi, Y. Kondo, K. Takayanagi, Nature (London) 395 (1998) 780.
- [10] F. Picaud, A. Dal Corso, E. Tosatti, Surf. Sci. 532-535 (2003) 544. [11] M. Michailov, D. Kashchiev, J. Phys. Conf. Ser. 398 (2012) 012010.
- [12] M. Michailov, D. Kashchiev, Physica E 70 (2015) 21-27.
- [13] F. Cleri, V. Rosato, Phys. Rev. B 48 (1993) 22.
- [14] M. Michailov, Phys. Rev. B 80 (2009) 035425.
- [15] M. Michailov, in: M. Michailov (Ed.), Nanophenomena at Surfaces: Funda-
- mentals of Exotic Condensed Matter Properties, Springer, Berlin, 2011, p. 145. [16] D.P. Landau, K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics, Cambridge University Press, Cambridge, 2000.

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