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Promoting the ordering of L1₀-FeNi phase via chemical interactions with substrate: A molecular dynamics simulation study

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ABSTRACT

The L1₀-type FeNi intermetallic phase is an important rare-earth-free magnetic material. However, its fabrication remains challenging. In this paper, we propose a chemical-interaction-enhanced ordering mechanism in vapor deposition processes, which is supported by molecular dynamics deposition simulations. Additionally, we describe guidelines for the fabrication of further ordered intermetallic thin films. Thus, we present not only the fabrication of an L1₀-type FeNi intermetallic magnet but also guidelines for developing diverse structural and functional layer-ordered intermetallic materials.

The L1₀-type FeNi intermetallic exhibits significant magnetic anisotropy and is anticipated to be a strong high-performance permanent magnet that does not require rare-earth elements [1,2]. However, the L1₀ phase that is in stable equilibrium at room temperature is observed only in the Fe-Ni alloy subjected to thermal histories under extremely slow-cooling conditions, such as those in meteorites, owing to the low order-disorder transformation temperature [3]. Consequently, fabricating L1₀-type FeNi intermetallics through conventional heat treatment is difficult; in this regard, innovative fabrication methods have been proposed, such as heating under neutron irradiation [4] and the dealloying of the Fe-Ni-N phase [5].

Recently, the formation of an L1₀ ordered phase has been reported in vapor-deposited FeNi thin films [6–10] and crystallized melt-spun ribbons [11,12]. In these studies, ordering was promoted by thermal stress due to the difference in thermal expansion between the deposited thin film and the substrate [13]. However, no ordering peak was observed in the samples that were heated while applying only stress to the bulk material using a ball mill [14], and the ordering mechanism must be elucidated.

We have recently come to notice that the formation of the ordered FeNi phase can be attributed to the elemental species in the substrate, similar to that of the ordering in the semiconductor thin films: Saito et al. reported [15] that the ordering of GeTe layered compounds in the

sputter-deposited films is promoted by the chemical interaction with the substrate and proposed that the ordering can be determined from the phase diagrams. Fig. 1 presents a periodic table colored according to the interactions with Fe or Ni based on the binary phase diagrams [16]. The L1₀-FeNi ordered domains are formed in sputtered thin films of FeNi on MgO, Cu buffer layers, Au-Cu-Ni, and Cu₄₀Ni₆₀ buffer layers [10]. The substrate elements, Mg, Cu, and Au, exhibit the opposite interactions with the Fe and Ni atoms. However, the L1₀ ordered peak cannot be observed in the diffraction patterns of FeNi films on the thermally oxidized amorphous Si substrates [17], which exhibit excellent interactions with both Fe and Ni atoms corresponding to the binary phase diagram. Additionally, the L1₀ ordered peaks can be observed in the diffraction patterns of the crystallized thin films containing the Cu [11] and C [12] atoms, which also exhibit opposite interactions with the Fe and Ni atoms (Fig. 1). Occurrence of ordering in the thin films due to chemical interactions has also been reported.

In this study, we determined the influence of chemical and physical interactions, i.e., the interactions caused by the difference in chemical identity of the substrate and by substrate-induced strain, respectively, between the atoms deposited on the substrates using molecular dynamics (MD) vapor deposition simulations. The simulations demonstrated that the chemical interactions facilitated the ordering of the L1₀-FeNi phase, whereas the physical interactions were ineffective.

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Additionally, we conducted simulations across various substrate temperatures (50–400 °C) to devise a strategy for achieving higher-order intermetallic thin films through the deposition process.

MD simulations were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [18]. The embedded atom method (EAM) potential, proposed by Bonny et al. [19,20], which considers the stability of the L1₀-FeNi intermetallic phase, was employed to model the interatomic interactions. Fig. 2a depicts the interatomic potential and geometry of the simulation model employed in this study. Ni and Cu were used as the substrates. The stable structure of both Ni (Fig. 2b1) and Cu (Fig. 2b2) at 25 °C comprise a face-centered cubic (fcc) structure in which the atomic positions are similar to that in the L1₀-FeNi phase (Fig. 2b3). Furthermore, Ni and Cu are expected to exhibit contrasting elemental preferences: Ni atoms attract the Fe atoms, whereas Cu atoms repel the Fe atoms, as indicated by the phase diagram (Fig. 1). Deposition on these substrates is expected to yield thin films with varied elemental distributions. The simulation domain was set to 30a₀ × 30a₀ × 50a₀, where a₀ denotes a lattice constant, and a₀ = 3.6149 Å and 3.524 Å for the Cu and Ni substrate models, respectively. A periodic boundary condition was applied along the x and y axes. Furthermore, simulations with different lattice constants and substrate temperatures were performed to determine an approach for obtaining higher-order intermetallic thin films via the deposition technique.

Initially, the Ni or Cu atoms were placed in the base 7a₀ of the domain to form the substrate (labeled substrate in Fig. 2a), and the uppermost 3a₀ of the substrate was maintained at 25 °C throughout the simulations (labeled moveable in Fig. 2a). A total of 5000 Fe atoms and 5000 Ni atoms were propelled from the center of the simulation domain with a constant velocity of 1.84 × 10³ m s⁻¹ (i.e., an average energy of 1.0 eV), which is characteristic of the sputtering process. The initial positions of the atoms along the x and y axes were randomized, with the z position was set at 35a₀. The ejection interval step was set to maintain the substrate temperature, as shown in Fig. 2c–d3. The ejected atoms traverse at a uniform velocity (Fig. 2d1), are drawn towards the substrate atoms (Fig. 2d2), and subsequently adhere and relax within 1.0 × 10⁻¹² s (1000 steps) (Fig. 2d3). Consequently, we deposited the film with an ejection time interval of 2.0 × 10⁻¹² s (2000 steps), exceeding the duration required for relaxation, since the movements of the stabilized atoms are negligible at the simulation temperatures. The deposited films were analyzed using the Open Visualization Tool (OVITO) [21], and the degree of ordering in the deposited films was assessed.

Fig. 3a presents the models of the FeNi thin films deposited on a Cu substrate, which was used as a representative example. The Cu, Fe, and Ni atoms are represented in red, blue, and yellow, respectively. During the simulations, the substrate temperature was maintained at 25 °C, resulting in the formation of a thin film comprising 50,000 atoms with an approximate thickness of 5 nm on both the substrates. To elucidate the impact of the substrate species differences on the element selectivity, we count the number N_i of i th neighboring Fe and Ni atoms from each substrate atoms on the surface, avoiding double counting with the deposited atoms which are counted for N_j ($j \leq i$). Fig. 3b and c illustrate the N_i of Fe and Ni atoms and Fig. 3d depicts the variation in the quantities of the Fe and Ni atoms. The selectivity trends for the Cu and Ni substrates are opposite. In the film deposited on the Ni substrate, the Fe atoms are more prevalent in the first-neighboring positions over the Ni atoms, which are more prevalent in the 3rd to 8th neighboring positions. Conversely, in the film deposited on the Cu substrate, Ni atoms are more prevalent in the first-neighboring positions, whereas Fe atoms are more prevalent in the 3rd to 8th neighboring positions. Fig. 3e depicts the temporal evolution of the degree of order of the first-neighboring position from the substrate atoms, S_1 , defined as $S_1 = (N_{1,Fe} - N_{1,Ni}) / (N_{1,Fe} + N_{1,Ni})$. The selectivity for the element at the first-neighboring position initially increased and then stabilized after 5 ns. The preferential selection of the nearest neighboring position is attributed to surface diffusion, driven by the intrinsic kinetic energy of the atom and the energy imparted by collisions with other atoms. Conversely, the opposite element selectivity occurs far beyond the nearest neighboring position. Our findings indicate that the chemical interactions between the deposited and substrate atoms induce this elemental selection. Elemental species with stronger attractive interactions are selectively positioned closest to the substrate, as shown schematically in Fig. 3f and g; that is, Ni atoms for the Cu substrate (Fig. 3f) and Fe atoms for the Ni substrate (Fig. 3g). This preferential placement facilitates the formation of a layered and ordered L1₀ structure, which is more likely to emerge than a random state by initiating from the ordered regions.

Extensive research has been conducted on intermetallic compounds with layer-like atomic configurations, such as the L1₀ and B2 structures, not only as structural materials [22–24], but also as functional materials [25–30]. It has been proposed that chemical interactions may contribute to the formation of intermetallic phases during the vapor deposition process. However, the chemical interactions cannot be determined

o: Forming a compound or Solid Solution x: Phase separation																					
■: Selective ■: Non-selective ■: No data available																					
H																	He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba	Ln	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				

Fig. 1. Periodic table of elements, color-coded to indicate the type of chemical interaction with Fe and Ni atoms, based on binary phase diagrams. The red color represents an interaction that is opposite to that of the Fe and Ni atoms, whereas the blue color indicates a similar type of interaction with both the Fe and Ni atoms.

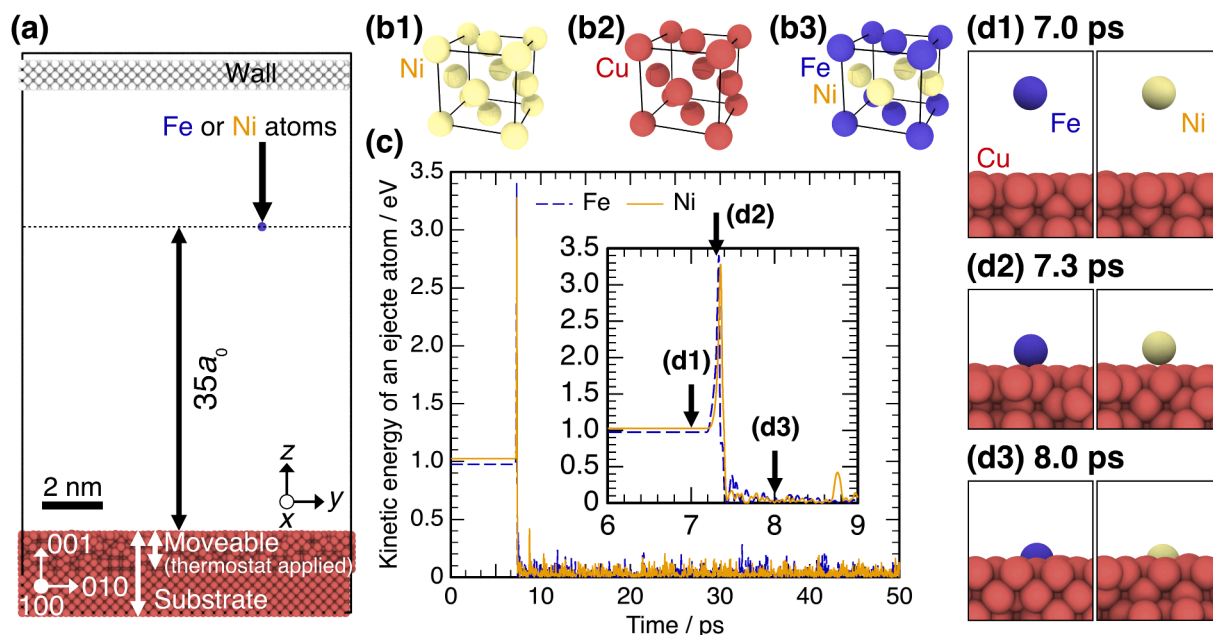


Fig. 2. (a) Side view of the MD simulation model. (b1–b3) Unit cells of Ni, Cu, and $L1_0$ -FeNi. (c) Kinetic energy profiles observed during the deposition of individual Fe or Ni atoms: snapshots at (d1) 7.0, (d2) 7.3, and (d3) 8.0 ps showing the positions of the ejected atoms.

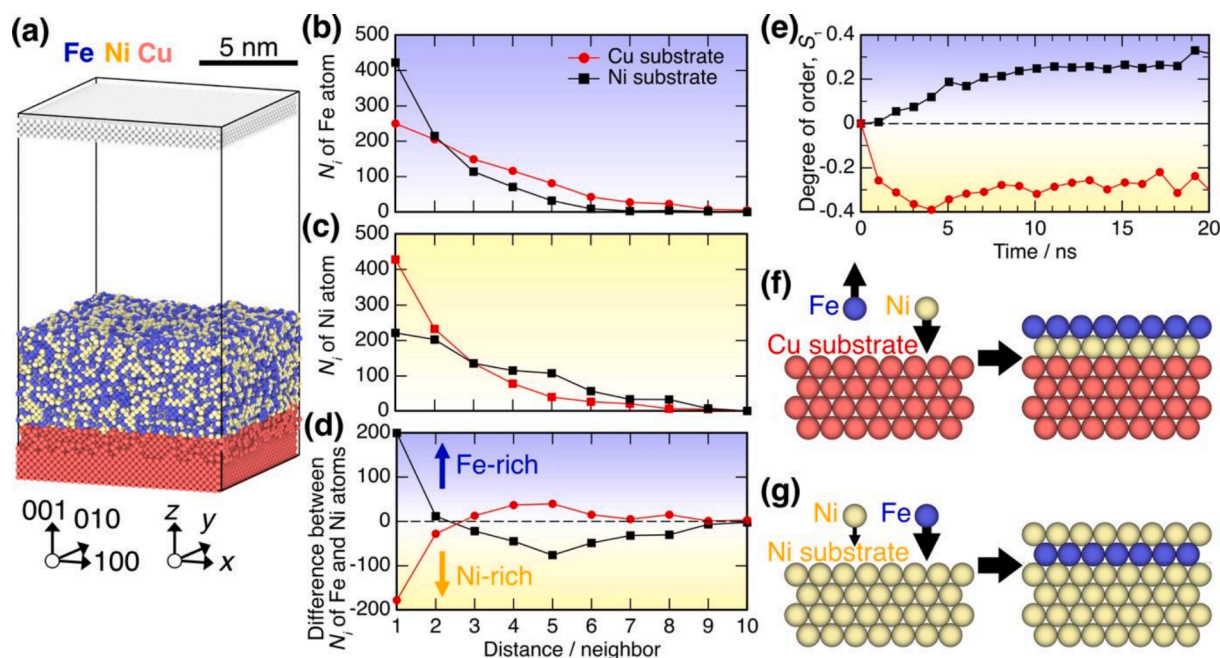


Fig. 3. (a) Side view of the simulation model of the FeNi thin films deposited on a Cu substrate. (b, c) Number of first to tenth nearest-neighbor Fe and Ni atoms from the substrate atoms, N_i , and (d) its numerical differences. (e) Change in the degree of order of the first-neighboring position from the substrate atoms, S_1 with respect to time. (f, g) Schematics of the selection of elements during the deposition process.

solely from the mixing enthalpy [31]. The mixing enthalpy values for Fe-Ni, Ni-Cu, and Fe-Cu are -2 kJ mol^{-1} , 4 kJ mol^{-1} , and 13 kJ mol^{-1} , respectively [31]. The magnitude of the Fe-Ni interaction (-2 kJ mol^{-1}) is less than the difference between those of Ni-Cu and Fe-Cu, which is 9 kJ mol^{-1} ; however, the degree of selectivity is nearly identical (Fig. 3b). Beyond the mixing enthalpy, the mixing entropy is also expected to contribute to the interaction and must be considered. Consequently, binary phase diagrams are proposed as a straightforward method for estimating the interactions.

We conducted deposition simulations using Cu and Ni substrates

with varying lattice constants to determine the effect of the physical substrate interactions, specifically the influence of lattice mismatch, on the ordering. Fig. 4 depicts the number of first-neighboring Fe and Ni atoms from the substrates and their differences. The quantities of both the Fe and Ni atoms increased with the increase in the lattice constants (Fig. 4a and b). The increase in the total number of the Fe and Ni atoms is supposed to be caused by the substrate-induced strain of the deposited FeNi thin film. The lattice constant of the deposited FeNi thin films onto the Ni substrates with lattice constants of Ni ($a_0 = 3.53 \text{ \AA}$) and FeNi ($a_0 = 3.58 \text{ \AA}$) are 3.53 \AA and 3.59 \AA , respectively. The lattice constants of the

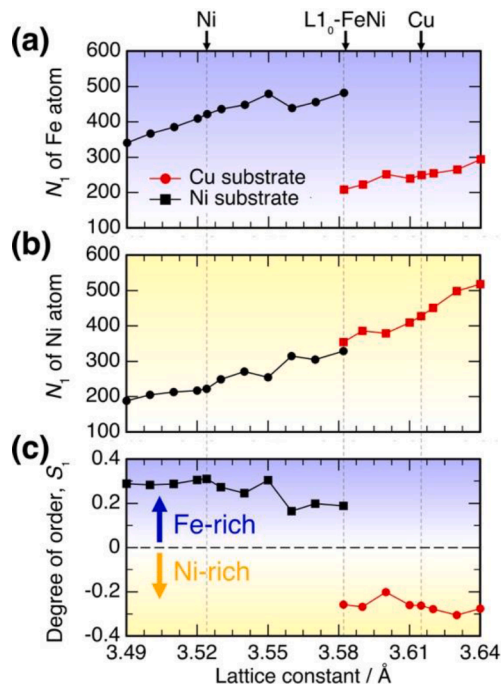


Fig. 4. Effect of lattice constant on the ordering behavior of thin films. (a,b) Number of the first nearest-neighbor Fe and Ni atoms, N_1 , deposited onto the substrates with various lattice constants, and (c) the degree of order of the first-neighboring position from the substrate atoms, S_1 .

deposited thin films are almost the same as that of the substrates. The compressive deposited layer is suggested to contain fewer sites to be occupied by the Fe and Ni atoms and cause the difference in the total number of the Fe and Ni atoms with the lattice constants. The degree of change with the increase in the lattice constants was nearly identical for

both the substrates (Fig. 4a and b) and no discernible differences were observed in the element selectivity corresponding to the lattice constants (Fig. 4c). This concurs with the experimental finding that stress application does not induce the ordering of the L1₀-FeNi phase [32]. These results suggest that chemical interactions have a more pronounced effect on the ordering behavior in the vapor deposition process than physical interactions. It is worth notably that Lewis and Stamenov [33] recently reported that the thermal treatment under stress and magnetic fields promotes the formation of the L1₀ FeNi phase in the bulk samples. In the present study, we suggested by the MD simulations that applying only the stress field does not promote the ordering. It is suggested that applying the magnetic field or the combination of stress and magnetic field is important for the development of the L1₀ ordering in FeNi alloy.

Subsequently, we analyzed the effect of the substrate temperature on the ordering behavior to obtain insights into the creation of more ordered intermetallic films. Fig. 5 depicts the number of Fe and Ni atoms in the first-neighboring positions of the substrates deposited at various substrate temperatures and the degree of order of the first-neighboring position from the substrate atoms, S_1 . The number of first-neighboring Fe atoms on the Ni substrate decreased with the increase in the substrate temperature (Fig. 5a–c). However, the number of first-neighboring Ni atoms on the Ni substrate and Fe and Ni atoms on the Cu substrates remained unaffected by the substrate temperature. Fig. 5d–f present the binary phase diagrams of the Cu-Fe [34], Cu-Ni [35], and Fe-Ni [36,37] systems. The Cu-Ni and Cu-Fe systems underwent the segregation and mixing of the Fe and Ni atoms (Fig. 5d and e); these interactions persisted at temperatures greater than the order–disorder transformation temperature of the L1₀-FeNi structure (Fig. 5f). These findings indicate that the substrates exhibiting distinct interactions with Fe and Ni at high temperatures exhibit greater chemical selectivity, even at higher temperatures, and promote ordering even under conditions of high substrate temperature, which encourages surface diffusions more frequently along with formations of ordered regions. Furthermore, it is reported that an even more ordered phase can

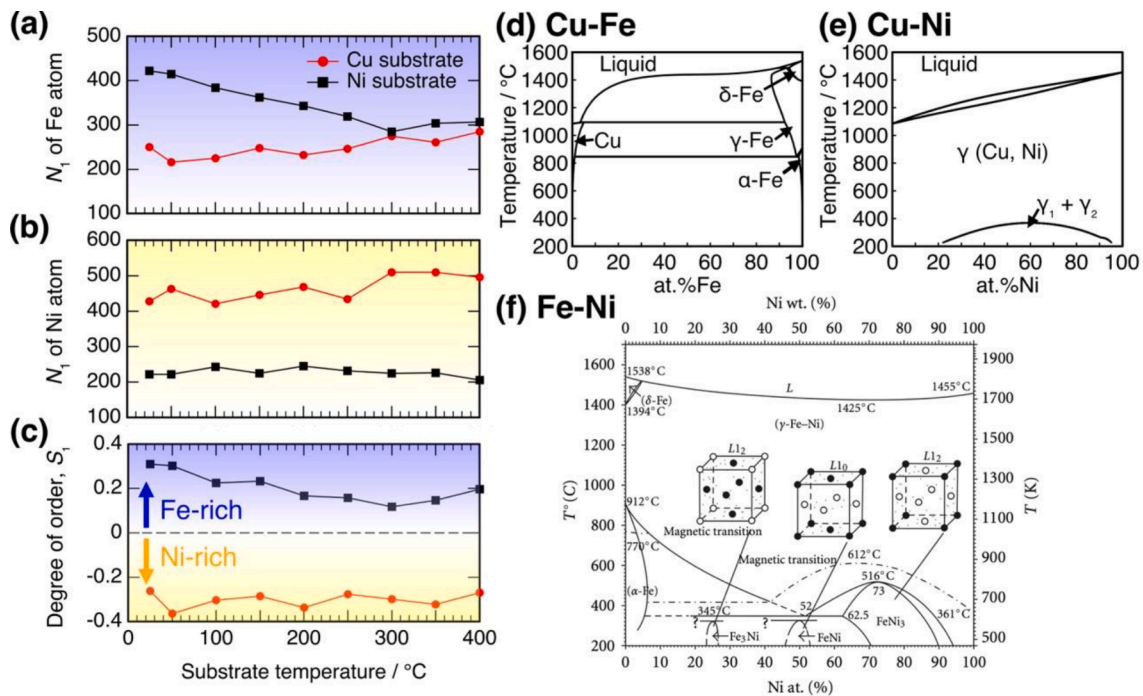


Fig. 5. Effect of substrate temperature on the ordering behavior of thin films. (a,b) Number of the first nearest-neighbor Fe and Ni atoms, N_1 , from the substrate atoms at various substrate temperatures. (c) the degree of order of the first-neighboring position from the substrate atoms, S_1 . (d–f) Binary phase diagrams for the Cu-Fe [34], Cu-Ni [35], and Fe-Ni [36,37] (taken from [Ref. 36]) under CC BY 3.0 DEED systems, showing the interactions between the elements at different temperatures.

be synthesized in the thin-film deposition process under high substrate temperature conditions by using a substrate that exhibits opposing interactions with the constituent elements at higher temperatures in binary phase diagrams.

In conclusion, we devised a novel chemical-interaction-enhanced ordering mechanism for the vapor deposition processes of the intermetallic alloy and corroborated it via MD simulations. We also analyzed the effects of the substrate lattice constant and substrate temperature on the ordering phenomena and proposed guidelines derived from binary phase diagrams to produce more ordered intermetallic thin films. This study highlights the role of chemical interactions in the ordering of intermetallic alloys and can contribute significantly to the advancement of sophisticated structural and functional layer-ordered intermetallic thin films.

Data availability statement

Data will be made available on request.

CRediT authorship contribution statement

Masayuki Okugawa: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Dmitri V. Louzguine-Luzgin:** Writing – review & editing, Validation, Project administration, Methodology, Conceptualization. **Yuichiro Koizumi:** Writing – review & editing, Validation. **Takeshi Nakanishi:** Writing – review & editing, Supervision, Project administration, Methodology.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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