Mechanical Resonance of embedded clusters

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Abstract

Embedded clusters, which are embedded in bulk materials and different from the surroundings in structures, should be common in materials. This paper studies resonance of such clusters. This work is stimulated by a recent experimental observation that some localized clusters behavior like fluid at the mesoscopic scale in many solid materials [Science in China(Series B). 46, 176 (2003)]. We argue that the phenomenon is just a vivid illustration of resonance of embedded clusters, driven by ubiquitous microwaves. Because the underlying mechanism is fundamental and embedded structures are usual, the phenomenon would have great significance in material physics.

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Mechanical resonance is a common thread which runs through almost every branch of physics. It occurs when the driving frequency matches the natural frequency of the sample. Recently, mechanical resonance has been observed at the mesoscopic scale for some nano-size materials. It takes place in near-field scanning optical microscope probes and some nanostructures such as carbon nanotubes, ZnO nanobelts, and SiO$_2$ nanowires. Mechanical resonance is a basic concept in textbooks and it is known that the boundary condition determines the normal modes of the samples. But theoretical analyses only cover samples with unambiguous boundaries, i.e., two fixed ends, two free ends, or one fixed end and one free end. Systematic knowledge is still lacking in such a typical case: embedded clusters, as shown in Fig. 1(a), which are embedded in a bulk material and are different from the surrounding parts in structure, and so have boundaries neither fixed nor free. This kind of clusters is usual at both macroscopic and mesoscopic scale in real world, such as materials embedded in other materials and the metastable structures in solids. It is clear that resonance can occur when the mechanical property of the embedded cluster is extremely different from that of surrounding materials and it can’t occur when the properties of the embedded cluster and the surrounding materials are quite similar. For general case, whether resonance can occur and how it occurs are still unclear.

The study of this problem is motivated by a recent experimental discovery of Gao et al. With an optical microscope, Gao et al. have observed some localized clusters in the range of 0.1×0.1µm$^2$ to 2×2µm$^2$ on the surface of a sample of Cu-Zn-Al alloy under normal pressure and temperature; these clusters behave like fluid: amorphism, flowing, waving, and they also expand and then contract; such motion can last from several seconds to several weeks. Later the similar phenomena have been observed in some other solid alloys, mineral crystal, gabbro, monocrystal nickel sulfate, semiconductor. In short, they find mesoscopic-scale clusters in many materials which show irregular movement at mesoscopic scale while their surroundings keep static. This is an interesting phenomenon and we believe that after the underlying mechanism is elucidated it will be recognized to be of significance and intensive studies will be focused. Our viewpoint is that the phenomenon is just a vivid illustration of resonance of the embedded clusters. The fluid-like clusters are metastable structures in solids and just embedded clusters referred above; ubiquitous microwaves can drive them into resonant vibrations when microwave frequencies match their natural frequencies; the
resonant vibrations can become marked movements at the mesoscopic scale if the sizes of the clusters and microwave intensities are appropriate.

For the sake of simplicity, we first employ a lattice as shown in Fig. 1(b) to study the resonance of the embedded cluster in a 1D sample. The Hamiltonian is

\[
H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2} + \frac{1}{2} \kappa_i (x_{i+1} - x_i)^2 + \frac{1}{4} \kappa_i (x_{i+1} - x_i)^4 \right]
\]

where \( p_i \) is the momentum of the \( i \)th atom, and \( x_i \) is the displacement from the equilibrium position. The mass \( m_i \) is set to unity and the first and last atoms are fixed. The force constant \( \kappa_i \) serves as the control parameter, which takes the value \( \kappa_o \) for \( i \in \left[ \frac{N-N_1}{2} + 1, \frac{N+N_1}{2} \right] \) and is set to unity for the other atoms. Then the middle part of the lattice with the \( N_1 \) atoms is structurally different from the other parts of the lattice and thus mimics the embedded cluster. The other parts represent the bulk sample. Notice that if \( \kappa_i \) is a constant for all atoms we will obtain the well-known Fermi-Pasta-Ulam model, which is a paradigm model in lattice studies.

For the embedded cluster, it is obvious that resonance can occur in the limit case of \( \kappa_o \to 0 \) (corresponding to fixed boundary condition) or \( \kappa_o \to \infty \) (to free boundary condition) when the driving frequency matches its nature frequency. As we know, the natural frequency is \( \omega_n = \frac{n \pi \sqrt{\kappa_o m}}{N_1} \cos \left( \frac{n \pi}{2N_1} \right) \) for both limit fixed and limit free boundary conditions, and the normal mode is \( x_n = A \sin(n \pi x_i / N_1) \) for the former and is \( x_n = A \cos(n \pi x_i / N_1) \) for the latter, where \( x_i \in \left[ \frac{N-N_1}{2} + 1, \frac{N+N_1}{2} \right] \). On the other hand, in the limit of \( \kappa_o \to 1 \) the embedded cluster appears indistinguishable with the other parts.

We apply numerical calculations to test whether resonance can occur in the embedded cluster in general case. In our simulations the first and last fifty atoms are coupled to Langevin thermostats\(^9\) which mimics the bulk sample in the environment temperature. The temperature \( T \) has been set equal to 0.01, corresponding to the room temperature.\(^10\) The thermodynamic equilibrium state is established after sufficient long evolutions, around \( t \sim 10^5 \). Then we apply periodic forces \( F = f \cos(\omega t) \) to the first fifty atoms, representing the driving forces applied on the surface of the bulk sample. In fig. 2(a) we show the average amplitude \( A \) of the embedded cluster versus the driving frequency \( \omega \) in the case of \( N = 3000, N_1 = 1000 \) and \( \kappa_o = 0.1 \). One can see, there are two maximum points at \( \omega_1 = 0.90 \times 10^{-3} \) and \( \omega_2 = 1.70 \times 10^{-3} \). From equation (1) we know that the first harmonic is
\( \omega'_1 = 1.0 \times 10^{-3} \) and the second harmonic is \( \omega'_2 = 2.0 \times 10^{-3} \) in theory for the embedded cluster with limit fixed or free boundary condition. The two maximum points \( \omega_1 \) and \( \omega_2 \) are close to the first and second harmonics respectively. Fig. 2(b) displays the vibration pattern of the lattice at \( \omega_1 \), and it is obvious that the pattern corresponds to the first normal mode of the embedded cluster in limit fixed boundary condition. We vary the value of \( \kappa_o \) to \( \kappa_o = 2 \). Resonance occurs at \( \omega = 4.6 \times 10^{-3} \), which is close to the theoretical value \( \omega'' = 4.4 \times 10^{-3} \). The vibration pattern (shown in Fig 2.(c)) agrees with the first normal mode of the embedded cluster in limit free boundary condition. Further calculations indicate that resonant mode at \( \kappa_o < 1 \) is similar to that at \( \kappa_o = 0.1 \) while resonant mode at \( \kappa_o > 1 \) is similar to that at \( \kappa_o = 2 \). These results indicate that resonance surely can occur in the embedded cluster when the force constant \( \kappa_o \) is sufficiently different from that of the surrounding part and resonance frequencies shift a little from the natural frequencies of embedded clusters with limit fixed or free boundary conditions.

Another notable is resonance amplitude. It is obvious that resonance amplitude \( A_f \) increases linearly with the magnitude \( f \) of the driving force. It is found that resonance amplitude also depend on the size of the embedded cluster. In Fig. 2(d) we plot \( A_f \) at the fundamental frequency versus \( N_1 \), and the curve shows \( A_f \) increases linearly with \( N_1 \). Moreover, \( A_f \) decreases with the increase of \( \kappa_o \) at \( \kappa_o < 1 \).

We extend the 1D lattice to a 2D lattice. Fig. 2 (e) and (f) show the vibration patterns at the fundamental frequency \( \omega = 0.026 \) and the second harmonic \( \omega = 0.041 \), which correspond to the first and second normal modes of the embedded cluster with limit fixed boundary condition respectively. In the calculation the 2D lattice size is \( 100 \times 100 \) and the embedded cluster at \( \kappa_o = 0.1 \) is \( 50 \times 50 \) in size.

So it is concluded that resonance can occur in embedded clusters if their force constants are sufficiently different from those of the surroundings and driving frequencies match their natural frequencies. In the following we illuminate the mechanism of Gao’s finding in detail. First we discuss whether there exist embedded clusters with quite different force constant in materials. We come to a simple three-atom model to achieve the relationship between the force constant \( \kappa \) and the atomic separation \( R \). Atoms \( a \) and \( c \) are fixed and atom \( b \) is connected to them. The atomic separation is \( R \). Supposing that the interactions between atoms are the Lennard-Jones
potential $U = \sigma^{12}R^{-12} - \sigma^{6}R^{-6}$, then the force constant of the atom $b$ is $\kappa(R) = -312\sigma^{12}R^{-14} + 84\sigma^{6}R^{-8}$. When the separation $R$ increases to 1.4 times (a larger change of lattice constant than 1.4 times has been observed in Gao's experiments), the force constant $\kappa_o$ decreases to about 0.06 times the initial one. Therefore, a little increase of atomic separation can lead to marked decrease of force constant and such embedded clusters can be extensive in materials.

From equation (1) the natural frequency of the embedded cluster can be estimated by 

$$\omega = \sqrt{\frac{\kappa_o}{m}} \cos \left(\frac{n\pi}{2N_1}\right) - \frac{1}{N_1\alpha} \sqrt{\frac{a^2 \rho}{m}} \cos \left(\frac{n\pi}{2N_1}\right) \quad v/l,$$

where $v$ verges on the sound velocity in the embedded cluster at around $10^3 m/s$ and $l$ verges on the size of the embedded cluster at from 0.1$\mu m$ to 2$\mu m$. Then the natural frequency is about $10^9 \sim 10^{10}$. It is obvious that in environment there exist external drives in the frequency range, such as ubiquitous microwaves.

Next we study whether the resonance amplitude of the embedded cluster can be large enough to be observed. Fig. 2(d) shows $A_f$ versus $N_1$ at $\kappa_o = 0.1$, $f = 0.01$ and $T = 0.01$. $A_f$ increases linearly with $N_1$ as $A_f \sim 0.14N_1$. We make an approximate correspondence between simulations and observations with the numerical result in fig. 2(d). For example, we obtain $A_f \sim 10^3$ at $N_1 \sim 10^4$. Then for such embedded cluster, the length is 1$\mu m$ and the resonance amplitude is about $10^2 nm$, supposing that the atomic separation 1 in the numerical simulations corresponds to 0.1 $nm$ in experiments. The value of the resonance amplitude is comparable to that observed in Gao’s finding. So resonance in the embedded cluster is observable with an optical microscope. Smaller localized clusters will be observed if the microscope has a larger magnification.

In summary, we investigate mechanical resonance in the embedded cluster. Resonance can take place when the structure of the embedded cluster is different enough from the surrounding material. Moreover, we believe Gao’s finding is resonance of embedded clusters at the mesoscopic scale of materials driven by ubiquitous microwaves. Embedded structures are common in solids, so the phenomenon would have great significance in material physics. Resonance in the embedded clusters may have influence on the thermodynamic properties at the macroscale and fracture at the mesoscopic scale of materials.

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Figure Captions

Fig. 1
(a). The embedded clusters. (b). The 1D lattice model.

Fig. 2
(a). The average amplitude $A$ versus the frequency $\omega$ of the external force. The values of the parameters are set as: $f = 0.01$, $\kappa_o = 0.1$, $N = 3000$ and $N_1 = 1000$. (b). The vibration pattern at $\omega = 0.80 \times 10^{-3}$. $\kappa_o = 0.1$. The $x$ axis is the site index ($i$) of the atom; the $y$ axis is the atom displacement from the equilibrium position. (c). The vibration pattern at $\omega = 4.8 \times 10^{-3}$. $\kappa_o = 2$. (d) $A_f$ versus the size $N_1$ of the embedded cluster. The values of the parameters are $f = 0.01$, $\kappa_o = 0.1$ and $N = 3 \times N_1$. (e) and (f). The two vibration patterns at the first and second harmonic of the 2D model. The $x$ and $y$ axes show the site index ($i,j$) of the atom; the $z$ axis shows the atom displacement from the equilibrium position. The lattice size is $100 \times 100$ and the embedded cluster size is $50 \times 50$. $\kappa_o = 0.1$. $f = 0.01$. $\omega_1 = 0.026$ and $\omega_2 = 0.041$.

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