Device Fatigue-fracture Caused by High Current Density
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Abstract—The electrons-migration under high current density can cause the distortion of molecules. The molecules deformation has two possible stable configurations when the electrons-migration is not symmetric in space. Geometrically, the non-symmetric electrons-migration behaves as a local rotation. When the electrons-migration is incompressible flow feature, the conductor may suffer fatigue effects, this is the normal case. However, when the electrons-migration is highly non-symmetric, only one stable configuration is possible, the conductor will produce fracture. The condition of fracture is described by an intrinsic parameter of critical local rotation angular, which is related with the yield stress of conductor material. This research gives the current density condition for the fatigue-fracture deformation. It shows that to increase the ability against the fatigue-fracture deformation, one can increase the critical angular of material (that is to say, increase the yield stress of material while at the same time reduce the elastic modulus). For fractured conductors, the current density will accelerate the fatigue-fracture process in the fractured position of conductor as it forms a high charge density there when the reference charge density is determined by initial or boundary condition.

1. INTRODUCTION
For VLSI devices, the high current density may produce fatigue-fracture although the current density is well among the limit of device-design. For electrical current induced fatigue-fracture problem, most researches put their attention on the mechanical aspects of material or thermo-mechanical features [1]. However, fracture mechanics predictions made using macroscopic material properties and a fatigue crack threshold of zero are not inconsistent with experiments [2]. Even for medium voltage motors, the experiments showed that mechanical stress or deformation is not enough to produce motor fatigue [3]. Therefore, the problem of fatigue-fracture caused by high current density get some attention recently. When the VLSI devices are largely used in electronic products, this problem should be given enough attention.

Usually speaking, the electrons-migration caused by high current density is uniform and is in parallel with the direction of current. However, when the boundary condition of conductors is put into consideration, this may not be so simple. Generally, even the distribution of conductor wires are symmetric, the instant current density may not be symmetric for high frequency current. So, the non-symmetric motion of electrons-migration should be studied.

The paper will firstly show that the non-symmetric electrons-migration behaves as a local rotation. Secondly, it goes to discuss under what geometrical condition the fatigue-fracture will appear. This leads to detailed discussion about the non-symmetric electrons-migration. After that, the related current density equation to describe such a kind of fatigue-fracture is introduced. Based on this formulation, the paper finally discusses how to evaluate the critical condition for the development of fatigue-fracture in electronic device.

2. GEOMETRIC MECHANICS OF ELECTRONS-MIGRATION
In molecule scale, the position of protons center can be taken to establish a local geometry of molecule. As the current produced by free electrons flows over the molecule, the electrons confined by the molecule structure will produce migration relative to the protons. Such a kind of electrons-migration will produce the distortion of molecules. This distortion, named as molecule deformation (hear after), can be formulated by a geometric field.

For the normal molecule when the current is zero, its position is coordinated by a standard rectangular system \((x^1, x^2, x^3)\). According to the structure theory of molecule, the confined electrons have their own quantum motion orbit. For a stable quantum state, the confined electrons form an electron cloud moving around the center of protons. Taking the position of molecule center \(\vec{r}\) as reference, the position representation of electron cloud can be expressed as \(\vec{\psi}_0(x)\), thus it behaves as a deterministic orbit round a fixed position:

\[
\vec{\psi}_0(x, t) = \vec{r} + \exp \left( \frac{iE}{\hbar} t \right) \cdot \vec{\psi}_0 dx^i
\] (1)
where, its quantum state function is $\sqrt{\det(g^0_{ij})} \cdot \exp(i\tilde{i}\theta)$, $\tilde{i}$ is imaginary sign, meets Schrödinger Equation [4], $E$ is the energy of electron cloud corresponding to a special orbit, $\theta$ is a phase item. $\vec{\psi}_0$ is the position of electron, $dx^i$ is the coordinator variants for the electron relative to the center of molecule, $\vec{g}^0_i$ are the initial base vectors in molecule scale. For a molecule, once it is defined on initial state, the coordinator will be fixed. By this way, the coordinator is rest on the center of molecule. Such a coordinator is named as co-moving dragging coordinator system. The initial size of molecule is given gauge field:

$$g^0_{ij} = \vec{g}^0_i \cdot \vec{g}^0_j$$  (2)

when free electrons pass through the molecule, the confined electrons are pushed to migrate a little. Hence, the molecule will deforms. That is described by the variation of the position representation of electron cloud.

$$\vec{\psi}(x, t) = \vec{r} + \exp\left(\frac{\tilde{i}E}{\hbar}t\right) \cdot \vec{g}_i(x)dx^i$$  (3)

Now the current base vectors are $\vec{g}_i(x)$, the determine the current size of molecule. Its current gauge field is:

$$g_{ij} = \vec{g}_i \cdot \vec{g}_j$$  (4)

Its quantum state function $\sqrt{\det(g_{ij})} \cdot \exp(i\tilde{i}\theta)$ meets Schrödinger Equation [4].

Geometrically, such a kind of molecule deformation can be expressed by transformation tensor $F^l_j$ defined as:

$$\vec{g}_i(x) = F^l_j(x)\vec{g}^0_j$$  (5)

As the position representation of electron cloud is continuous on the measure of probability, covariant differentiation can be introduced. Under this understanding, the molecule deformation can be expressed as the finite deformation of continuum.

By Equations (2), (4) and (5), it is found that:

$$g_{ij} = F^k_i F^l_j g^0_{kl}$$  (6)

For continuum, the deformation tensor $F$ is related with macro displacement (distance variation) field $U^i$. For an idea unit material element, without the lose of generality, supposing the number of molecules in the unit material element is $N$, and the molecules are homogeneously distributed, then one will have:

$$\sum_N g^{0N}_{ij} = \sum_N F^{kN}_i F^{lN}_j \delta^{0N}_{kl} = F^{kN}_i F^{lN}_j \sum_N g_{kl}^{0N}$$  (7)

where, upper index $N$ represents the sequence number of molecules. For simplicity, the initial material is supposed as isotropic, and hence one has:

$$\sum_N g_{kl}^{0N} = \delta_{ij}$$  (8)

Therefore, the current material will have a macro gauge field as:

$$G_{ij} = \sum_N g^{0N}_{ij} = F^{kN}_i F^{lN}_j \sum_N g_{kl}^{0N} = F^{kN}_i F^{lN}_j$$  (9)

For continuum, for a given displacement field $U^i$, the deformation tensor is defined as:

$$F^i_j = \frac{\partial U^i}{\partial x^j} + \delta^i_j$$  (10)

For idea simple elastic material, the corresponding stress field is:

$$\sigma^i_j = \lambda(F^i_j - 3)\delta^i_j + 2\mu(F^i_j - \delta^i_j)$$  (11)

Therefore, the molecule deformation is related with the macro deformation of material.
3. FEATURE OF DEFORMATION TENSOR

In geometrical field theory, for a continuous displacement field, the deformation tensor can decompose as the addition of a symmetric tensor and an orthogonal rotation tensor [5]:

\[ F^i_j = S^i_j + \frac{1}{\cos \Theta} R^i_j \]  

where,

\[ S^i_j = \frac{1}{2} \left( U^i_j + U^i_j^T \right) - \left( \frac{1}{\cos \Theta} - 1 \right) \left( L^i_k L^k_j + \delta^i_j \right) \]  

\[ \frac{1}{\cos \Theta} R^i_j = \delta^i_j + L^i_j \frac{\sin \Theta}{\cos \Theta} + \left( \frac{1}{\cos \Theta} - 1 \right) \left( L^i_k L^k_j + \delta^i_j \right) \]  

\[ L^i_j = \frac{\cos \Theta}{2 \sin \Theta} \left( U^i_j - U^i_j^T \right) \]  

\[ \cos^{-2} \Theta = 1 + \frac{1}{4} \left[ \left( U^1|_2^2 - U^2|_1^2 \right)^2 \right. \\
\left. + \left( U^2|_3^2 - U^3|_2^2 \right)^2 + \left( U^3|_1^2 - U^1|_3^2 \right)^2 \right] \]  

\[ \Theta \] represents the local rotation angular, \( L^i_j \) represents the unit vector along the rotation axis, \( R^i_j \) is an unit orthogonal rotation tensor, upper index \( T \) represents transpose. Note that when there is no displacement gradient, \( F^i_j = \delta^i_j \).

Consider the mass conservation requirement of motion:

\[ \frac{\partial m}{\partial t} + \nabla m \cdot \vec{v} + m \nabla \cdot \vec{v} = 0 \]  

here, \( m \) represents the mass density, \( \vec{v} \) is the velocity of electrons migration.

Geometrically, there is a relation equation between the initial and current configurations:

\[ m \sqrt{g} = m_0 \sqrt{g^0} \]  

where, \( g = \det(g_{ij}) \), \( g^0 = \det(g^0_{ij}) \). Hence, one has:

\[ \frac{\partial}{\partial t} \left( \frac{1}{\sqrt{g}} \right) + \nabla \left( \frac{1}{\sqrt{g}} \right) \cdot \vec{v} + \left( \frac{1}{\sqrt{g}} \right) \nabla \cdot \vec{v} = 0 \]  

It has two typical solutions. One solution is:

\[ g_{ij} = \delta_{ij}, \quad \nabla \cdot \vec{v} = 0 \]  

It corresponds to the incompressible fluid model of electrons migration. It usually leads to thermal mechanics interpretation.

Another solution is:

\[ g_{ij} = \frac{1}{\cos^2 \Theta} \delta_{ij} \]  

For such a kind of deformation, one has: \( S^i_j = 0 \) and:

\[ F^i_j = \frac{1}{\cos \Theta} R^i_j \]  

Therefore, the molecule has volume variation:

\[ \delta = \frac{1}{\cos \Theta} - 1 \]  

That means the fatigue-fracture has been appeared in material.
For the former solution \( g_{ij} = \delta_{ij}, \nabla \cdot \vec{V} = 0 \), it is possible only when the following condition is met:

\[
1 > \frac{1}{4} \left[ (U^1|_2 - U^2|_1)^2 + (U^2|_3 - U^3|_2)^2 + (U^3|_1 - U^1|_3)^2 \right]
\]

In this case, there is another decomposition of deformation [6]:

\[
F_{ij} = \tilde{S}_{ij} + \tilde{R}_{ij}
\]

where,

\[
\tilde{S}_{ij} = \frac{1}{2} \left( U^i|_j + U^i|_j^T \right) - (1 - \cos \tilde{\Theta}) \tilde{L}_k L_j^k
\]

\[
\tilde{R}_{ij} = \delta_{ij} + \sin \tilde{\Theta} \cdot \tilde{L}_j + (1 - \cos \tilde{\Theta}) \tilde{L}_k L_j^k
\]

\[
\sin^2 \tilde{\Theta} = \frac{1}{4} \left[ (U^1|_2 - U^2|_1)^2 + (U^2|_3 - U^3|_2)^2 + (U^3|_1 - U^1|_3)^2 \right]
\]

The solution is:

\[
\tilde{S}_{ij} = 0 \quad F_{ij} = \tilde{R}_{ij}
\]

For such a kind of deformation, no fatigue-fracture is produced. The deformation is pure elastic.

Based on classical mechanics, the strain for fatigue-fracture deformation is:

\[
\varepsilon_{ij} = \left( \frac{1}{\cos \Theta} - 1 \right) (L_k L_j^k + \delta_{ij})
\]

as comparing the strain for pure elastic deformation is:

\[
\varepsilon_{ij} = (1 - \cos \tilde{\Theta}) \tilde{L}_j L_j^k
\]

For fatigue-fracture rotation along \( x^3 \) axis, \( L_2^1 = -L_1^2 = 1 \), other \( L_j^i = 0 \):

\[
\varepsilon_3^3 = \frac{1}{\cos \Theta} - 1, \quad \text{others are zero}
\]

Therefore, the molecule has elongation along the rotation axis. For such a kind of deformation, excepting the isotropic stress \( \lambda \left( \frac{1}{\cos \Theta} - 1 \right) \delta_{ij} \), there are an additional stress component along the rotation axis \( \sigma_{33} = 2\mu \left( \frac{1}{\cos \Theta} - 1 \right) \). Therefore, the maximum stress is along the rotation axis direction.

For pure elastic rotation along \( x^3 \) axis, \( \tilde{L}_2^1 = -\tilde{L}_1^2 = 1 \), other \( \tilde{L}_j^i = 0 \):

\[
\varepsilon_3^3 = \varepsilon_2^2 = 1 - \cos \tilde{\Theta}, \quad \text{others are zero}
\]

It is a pure rigid rotation. For such a kind of deformation, excepting the isotropic stress \( \lambda(1 - \cos \tilde{\Theta})\delta_{ij} \), there are additional plane stress on the rotation plane \( \sigma_{11} = \sigma_{22} = 2\mu(1 - \cos \tilde{\Theta})\delta_{ij} \). Therefore, the minimum stress is along the rotation axis direction.

Generally speaking, for a given material, there exists an intrinsic parameter of material \( \Theta_c \), when:

\[
\Theta \geq \Theta_c
\]

only fatigue-fracture deformation solution can exist. This topic is well known in plasticity theory for the yield condition. The yield stress and the critical rotation angular for simple elastic material has relation equation: \( \sigma_S = (\lambda + 2\mu)(1 - \cos \Theta_c), (\cos \Theta_c)^{-2} = 1 + \sin^2 \tilde{\Theta}_c \). The detailed discussion is out the range of this paper, hence is omitted here.
4. CRITICAL CURRENT DENSITY FOR FATIGUE-FRACTURE DEFORMATION

For fatigue-fracture deformation, as the deformation meets Equations (19) and (22), after simple algebra operation, one has:

\[ \frac{\partial}{\partial t} \cos \Theta + \nabla \cos \Theta \cdot \vec{V} + \cos \Theta \cdot \nabla \cdot \vec{V} = 0 \]  

(36)

Ignoring the space variation of local rotation, it can be approximated as:

\[ \frac{\partial}{\partial t} \cos \Theta + \cos \Theta \cdot \nabla \cdot \vec{V} = 0 \]  

(37)

For a given \( \Theta \) harmonic motion with intrinsic frequency \( \tilde{\omega} \), (which is determined by the quantum state function of molecules, it is an intrinsic parameter of material structure), its form is:

\[ \nabla \cdot \vec{V} = \tilde{\omega} \cdot \tan \Theta \]  

(38)

Based on discussion in last section, when the local rotation angular is bigger than the material critical value, that is when: Equation (35) \( \Theta \geq \Theta_c \) is met. The only possible deformation is fatigue-fracture type. This condition can be expressed as:

\[ \nabla \cdot \vec{V} \geq \tilde{\omega} \cdot \tan \Theta_c \]  

(39)

It gives the upper limit for the current density as: \( \vec{J} = \rho \vec{V} \), for a constant charge density, one has:

\[ \nabla \cdot \vec{J} \geq \rho \tilde{\omega} \cdot \tan \Theta_c \]  

(40)

This equation gives the current density condition for the fatigue-fracture deformation. It shows that to increase the ability to against the fatigue-fracture deformation, one can increase the critical angular \( \Theta_c \) of material (that is to say, increase the yield stress of material while at the same time reduce the elastic modulus), or increase the intrinsic frequency of molecules \( \tilde{\omega} \), or increase charge density \( \rho \). Theoretically, one has \( \tilde{\omega} = \frac{\tilde{E} - E}{\hbar} \), if both Schrödinger equations for initial state and current state are met. This parameter usually is discussed by statistical method to relate with temperature. So, here it can be understood as a thermal parameter.

5. CURRENT DENSITY IN FRACTURED CONDUCTOR

Once the fatigue-fracture deformation is produced in conductors, it does not mean that the device will break down at once. So, it is meaningful to discuss the current density in fractured conductors.

Using \( \vec{V}_P \) to represent the charge velocity of conductor, then for the fractured conductor, one has:

\[ \nabla \cdot \vec{V}_P = \frac{1}{\cos \Theta} - 1 \]  

(41)

The charge conservation equation gives:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{V}_P \rho \nabla \cdot \vec{V}_P = 0 \]  

(42)

where, \( \rho \) is charge density. Putting Equation (41) into (42), letting \( \frac{\partial \rho}{\partial t} = \omega \cdot a(t) \cdot \rho \), one gets:

\[ \nabla \cdot \vec{V}_P = - \left[ \left( \frac{1}{\cos \Theta} - 1 \right) + \omega \cdot a(t) \right] \rho \]  

(43)

Its solution in form is:

\[ \rho = \rho_P \cdot \exp \left\{ \left[ -A(\Theta, \omega, t) \right] \cdot \vec{k} \cdot d\vec{r} \right\} \]  

(44)

where, \( \vec{k} \) is a unit vector along the velocity direction, that in fact is the local rotation axis direction, and the parameter is:

\[ A(\Theta, \omega, t) = \left( \frac{1}{\cos \Theta} - 1 \right) + \omega \cdot a(t) \]  

(45)
For the fracture produced by local rotation along $x^3$ direction, taking the center position of conductor as reference point for charge density, the current density is:

$$J_P = \tilde{\rho}_P \cdot \exp\left\{ -A(\Theta, \omega, t)/V_P \right\} \cdot x^3 \cdot V_P$$  \hspace{1cm} (46)

Hence, the current density will accelerate the fatigue-fracture process in the fractured position of conductor as it forms a high charge density there when the reference charge density $\tilde{\rho}_P$ is determined by initial or boundary condition. It is very interesting to notice that once the fracture is produced in conductor, the higher frequency will accelerate the further development of fracture, and therefore accelerates the breakdown of device.

Generally, highly non-symmetric electrons-migration appears only when there is a body force. Such a kind of body force may be produced by: the magnetic field produced by high frequency current which may be related with bad layout of wires, the non-symmetric stress acting on the conductor which may be related with bad geometry of device packing, and the anisotropic thermal expansion related with the cooling system. The research shows the geometric feature of fatigue-fracture. For a suitable design, the damage caused by the fracture effects can be reduced theoretically.

REFERENCES