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Marek Danielewski[1], Lucjan Sapa[2]

[1]Faculty of Materials Science and Ceramics, AGH University of Science and Technology
Mickiewicza 30, 30-059 Kraków, Poland. E-mail: daniel@agh.edu.pl
[2]Faculty of Applied Mathematics, AGH University of Science and Technology

NONLINEAR KLEIN-GORDON EQUATION IN CAUCHY-NAVIER ELASTIC SOLID

We show that the quaternionic field theory can be rigorously derived from the classical balance equations in an isotropic ideal crystal where the momentum transport and the field energy are described by the Cauchy-Navier equation. The theory is presented in the form of the non-linear wave and Poisson equations with quaternion valued wave functions. The derived quaternionic form of the Cauchy-Navier equation couples the compression and torsion of the displacement. The wave equation has the form of the nonlinear Klein-Gordon equation and describes a spatially localized wave function that is equivalent to the particle. The derived wave equation avoids the problems of negative energy and probability. We show the self-consistent classical interpretation of wave phenomena and gravity.

Keywords: quantum wave, quaternion algebra, Klein-Gordon equation, gravity.

1. Introduction

In 1821 Navier formulated the general theory of elasticity [1], "*A Dynamical Theory of the Electromagnetic Field*" was published by Maxwell in 1856 [2]. The hypothesis that we make use of in this work can be found in his paper. Let us begin with the well-known Maxwell remark on the ether [2]:

"On our theory it (energy) resides in the electromagnetic field, in the space surrounding the electrified and magnetic bodies, as well as in those bodies themselves,… may be described… according to a very probable hypothesis, as the motion and the strain of one and the same medium (elastic ether)".

In the almost unnoticed part of his paper, Maxwell wrote:

"…assumption, therefore, that gravitation arises from the action of the surrounding medium… leads to the conclusion that every part of this medium possesses, when undisturbed, an enormous intrinsic energy… As I am unable to understand in what way a medium can possess such properties, I cannot go any further in this direction in searching for the cause of gravitation."

The properties of *such a medium* are presented in Table 1. Maxwell's hypothesis was already investigated [3, 4], but connection with quantum mechanics was incomplete [5]. The first basis for relativistic quantum mechanics was found by Klein in 1926 and it is known as the Klein–Gordon equation, KGE [6]. Dirac maintained that the KGE equation is unacceptable [7] throughout his life.

Basing on the Maxwell hypothesis [2] we combine the theory of elasticity [1] and the quaternion algebra discovered by Hamilton in 1843 [8]. Quaternion formulation of the elasticity theory allows expressing momentum conservation in the Klein form of the wave equation [6] and the Poisson equation. Quaternion formalism allows analyzing such phenomena [11]. Properties of the medium (crystal) are shown in Table 1. For simplicity, we consider the small deformation limit and consequently neglect here the effects due to density changes.

Table 1

The physical constants of the ideal isotropic crystal.

Physical Quantity	Unit	Symbol for unit	Value	SI unit	Reference
Lattice parameter	Planck length	l_P	$1.616229(38)\cdot 10^{-35}$	m	[9]
Poisson ratio		ν	0.25	-	[10]
Mass of particle	Planck mass	m_P	$2.176470(51)\cdot 10^{-8}$	kg	[9]
Planck density	Mass density	ρ	$2.062072\cdot 10^{97}$	$kg\cdot m^{-3}$	[9]
Duration of the internal process	Planck time	t_P	$5.39116(13)\cdot 10^{-44}$	s^{-1}	[9]
Young modulus	Energy density	Y	$4.6332447\cdot 10^{114}$	$kg\cdot m^{-1}\cdot s^{-2}$	This work

2. The quaternion representation of the deformation field

The Navier-Cauchy momentum equation in an elastic solid shows coupling between compression and torsion in the displacement $\mathbf{u}\in\mathbb{R}^3$. Coupling becomes evident in the boundary condition (nonlocal) for the suitable differential equations on the quaternionic deformation field $\sigma=\sigma_0+\hat{\phi}\in H$, where symbol H denotes the quaternion algebra, $\sigma_0=\operatorname{div}\mathbf{u}_0$, $\hat{\phi}=\operatorname{rot}\mathbf{u}_\phi$ and $\mathbf{u}=\mathbf{u}_0+\mathbf{u}_\phi$.

In the isotropic crystal (Poisson number $\nu=0.25$) the displacement $\mathbf{u}\in\mathbb{R}^3$ is described by

$$\frac{\partial^2\mathbf{u}}{\partial t^2} = 3\frac{0.4Y}{\rho}\operatorname{grad}\operatorname{div}\mathbf{u} - \frac{0.4Y}{\rho}\operatorname{rot}\operatorname{rot}\mathbf{u}, \tag{1}$$

where Y and ρ denote the Young modulus and density shown in Table 1.

From Eq. (1), the local energy density in the deformation field follows [1]

$$e=\frac{1}{2}\dot{\mathbf{u}}\circ\dot{\mathbf{u}}+\frac{3}{2}\frac{0.4Y}{\rho}\left(\operatorname{div}\mathbf{u}\right)^2+\frac{1}{2}\frac{0.4Y}{\rho}\operatorname{rot}\mathbf{u}\circ\operatorname{rot}\mathbf{u}, \tag{2}$$

where $\dot{\mathbf{u}}=\partial\mathbf{u}/\partial t$ and $\circ$ is the standard product in $\mathbb{R}^3$

In the small deformation limit $Y/\rho\cong const$, and one gets equivalently

$$\frac{\partial^2\mathbf{u}}{\partial t^2}=3c^2\operatorname{grad}\operatorname{div}\mathbf{u}-c^2\operatorname{rot}\operatorname{rot}\mathbf{u}, \tag{3}$$

$$e=\frac{1}{2}\dot{\mathbf{u}}\circ\dot{\mathbf{u}}+\frac{1}{2}c^2\left(\operatorname{div}\mathbf{u}\right)^2+\frac{1}{2}c^2\operatorname{rot}\mathbf{u}\circ\operatorname{rot}\mathbf{u}+c^2\left(\operatorname{div}\mathbf{u}\right)^2, \tag{4}$$

where the Young modulus was estimated from the velocity of the transverse wave: $c=\sqrt{0.4Y/\rho}=2.99792458\cdot 10^8$.

Every deformation can be expressed by compression and rotation, i.e., can be divided into an irrotational and a solenoidal component. Thus, let $\mathbf{u}$ belongs to the C^3 class of functions. By the Helmholtz decomposition theorem: $\mathbf{u}=\mathbf{u}_0+\mathbf{u}_\phi$, $\operatorname{rot}\mathbf{u}_0=0$ and $\operatorname{div}\mathbf{u}_\phi=0$, the Eq. (3) and formula (4) become

$$\frac{\partial^2}{\partial t^2}\left(\mathbf{u}_0+\mathbf{u}_\phi\right)=2c^2\operatorname{grad}\operatorname{div}\mathbf{u}_0+c^2\,\Delta\left(\mathbf{u}_0+\mathbf{u}_\phi\right), \tag{5}$$

$$e=\frac{1}{2}\dot{\mathbf{u}}\circ\dot{\mathbf{u}}+\frac{1}{2}c^2\left[\left(\operatorname{div}\mathbf{u}_0\right)^2+\operatorname{rot}\mathbf{u}_\phi\circ\operatorname{rot}\mathbf{u}_\phi\right]+c^2\left(\operatorname{div}\mathbf{u}_0\right)^2. \tag{6}$$

Thus, there existsa deformation field σ, such that one can represent the solenoidal (vector) and irrotational
(scalar) fields as a superposition of the real and imaginary field parts at each point. From (5) and (6)

$$\begin{aligned}\sigma&=\sigma_0+\hat{\phi}\quad\in H,\\ \sigma^*&=\sigma_0-\hat{\phi}\quad\in H,\end{aligned} \tag{7}$$

Where H denotes the quaternion algebra [11], $\sigma_0=\operatorname{div}\mathbf{u}_0$, $\hat{\phi}=\operatorname{rot}\mathbf{u}_\phi$, $\operatorname{div}\hat{\phi}=\operatorname{div}\operatorname{rot}\mathbf{u}_\phi=0$ and $\hat{\phi}=\phi_1\,\mathbf{i}+\phi_2\,\mathbf{j}+\phi_3\,\mathbf{k}$, where **i, j, k** are the quaternion imaginary units obeying the following relations:

$$\begin{aligned}&\mathbf{i}^2=\mathbf{j}^2=\mathbf{k}^2=-1,\quad \mathbf{ij}=-\mathbf{ji}=\mathbf{k},\\ &\mathbf{jk}=-\mathbf{kj}=\mathbf{i},\qquad \mathbf{ki}=-\mathbf{ik}=\mathbf{j}.\end{aligned} \tag{8}$$

Because $\mathbf{u}$ belongs to the $\mathbb{C}^3$ class, and upon acting on Eq. (5) by the rotation and divergence operators, we can express it by the system

$$\begin{cases}\dfrac{\partial^2\hat{\phi}}{\partial t^2}=c^2\Delta\hat{\phi},\\[2ex] \dfrac{\partial^2\sigma_0}{\partial t^2}=3c^2\,\Delta\sigma_0.\end{cases} \tag{9}$$

The local energy density of the deformation field per mass unit, formula (6), is now expressed by

$$e=\tfrac{1}{2}\hat{\dot{\mathbf{u}}}\circ\hat{\dot{\mathbf{u}}}+\tfrac{1}{2}c^2\;\sigma\cdot\sigma^*+c^2\sigma_0^2, \tag{10}$$

where $\hat{\dot{\mathbf{u}}}=\dot{u}_1\,\mathbf{i}+\dot{u}_2\,\mathbf{j}+\dot{u}_3\,\mathbf{k}$. By adding Eqs. (9) and from (7), the system (9) is expressed by a single partial differential equation:

$$\frac{\partial^2\sigma}{\partial t^2}=c^2\Delta\sigma+2c^2\Delta\sigma_0. \tag{11}$$

In the next section we will show that upon splitting Eq. (11) into the system of wave and Poisson equations, the nonlinear form of the wave equation follows.

3. From the quaternion equation of motion to nonlinear wave and Poisson equations

We consider a stationary wave, $m=Ec^{-2}=const$. Thus, Eq. (11) can be written as a system:

$$\begin{cases}\left(\dfrac{\partial^2}{\partial t^2}-c^2\Delta+\dfrac{8\pi m}{m_P t_P^2}\sigma^*\right)\sigma=0,\\[2ex] 2c^2\Delta\sigma_0=-\dfrac{8\pi m}{m_P t_P^2}\sigma\cdot\sigma^*.\end{cases} \tag{12}$$

The wave equation in (12) can be written in the more compacted form

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\Delta\right)\sigma+\frac{8\pi m}{m_P\,c^2 t_P^2}\sigma^*\cdot\sigma=0, \tag{13}$$

or in the covariant notation

$$\partial_\mu \partial^\mu \sigma + m \frac{8\pi}{\hbar t_P} \sigma^* \cdot \sigma = 0, \tag{14}$$

where $\partial_\mu \partial^\mu = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta$ and $\hbar = m_P c^2 t_P = 1.0545727 \cdot 10^{-34} \left[\text{kg m}^2\text{s}^{-1}\right]$.

The wave equation in the most compacted form is given by

$$\left(\partial_\mu \partial^\mu + m \ell_P \sigma^*\right) \cdot \sigma = 0 \tag{15}$$

where $\ell_P = 8\pi \big/ \left(m_P l_P^2\right) = 4.4205986 \cdot 10^{78} \left[\text{kg}^{-1}\text{m}^{-2}\right]$.

System (12) is a hyperbolic-elliptic quaternion representations of a wave equation (11) and has solution of the form:

$$\sigma = \sigma_0 + \hat{\phi} = \sigma_0 + \phi_1 \mathbf{i} + \phi_2 \mathbf{j} + \phi_3 \mathbf{k} \in H. \tag{16}$$

The second equation in (12) is the Poisson equation and describes the irrotational, e.g., compression, potential in the deformation field

$$c^2 \Delta \sigma_0 = -4\pi m \frac{1}{m_P t_P^2} \sigma \cdot \sigma^*, \tag{17}$$

it can be expressed as a function of the local mass density: $\rho = m\sigma \cdot \sigma^* / l_P^3$. Thus (17) becomes:

$$c^2 \Delta \sigma_0 = -4\pi\rho \frac{l_P^3}{m_P t_P^2} = -4\pi \rho G, \tag{18}$$

using data in Table 1, the gravitational constant equals: $G = l_P^3 \big/ \left(t_P^2 m_P\right) = 6.674082 \cdot 10^{-11} \left[\text{m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}\right]$. Equations (9)-(15) require boundary conditions for a solution.

4. The additional integral equation

The energy is conserved thus, for $t \geq 0$ from Eq. (10) follows

$$\int_{\mathbb{R}^3} \left(\frac{1}{2} \hat{\mathbf{u}} \circ \hat{\mathbf{u}} + \frac{1}{2} c^2 \, \sigma \cdot \sigma^* + c^2 \sigma_0^2 \right) \mathrm{d}^3 \mathbf{r} = const. \tag{19}$$

In a case of the bounded closed volume $\Omega \subset \mathbb{R}^3$, the above energy conservation formula becomes

$$\int_{\Omega} \left(\frac{1}{2} \hat{\mathbf{u}} \circ \hat{\mathbf{u}} + \frac{1}{2} c^2 \, \sigma \cdot \sigma^* + c^2 \sigma_0^2 \right) \mathrm{d}^3 \mathbf{r} = \frac{E(\Omega)}{m_P} = \frac{mc^2}{m_P},$$

$$\int_{\Omega} \left(\frac{m_P}{2c^2} \hat{\mathbf{u}} \circ \hat{\mathbf{u}} + \frac{1}{2} m_P \sigma \cdot \sigma^* + m_P \sigma_0^2 \right) \mathrm{d}^3 \mathbf{r} = m(\Omega). \tag{20}$$

The integral (20) can be treated as a **nonlocal boundary condition** for Eqs. (11)-(15).

5. The nonlocal boundary condition

In order to obtain a more simple and useful nonlocal boundary condition, the formula for the local energy density (4), should be expressed by the local energy flux S in the continuity equation

$$\frac{\partial e}{\partial t} + \operatorname{div} S = 0. \tag{21}$$

Below we derive the quaternion form of the energy flux following the Cauchy schema. Formula (4) upon differentiation becomes

$$\frac{\partial e}{\partial t} = \dot{\mathbf{u}} \circ \ddot{\mathbf{u}} + 3c^2 \operatorname{div}\mathbf{u} \operatorname{div}\dot{\mathbf{u}} + c^2 \operatorname{rot}\mathbf{u} \circ \operatorname{rot}\dot{\mathbf{u}} \tag{22}$$

and using Eq. (3) we have

$$\frac{\partial e}{\partial t} = \dot{\mathbf{u}} \circ \left(3c^2 \operatorname{grad}\operatorname{div}\mathbf{u} - c^2 \operatorname{rot}\operatorname{rot}\mathbf{u}\right) + 3c^2 \operatorname{div}\mathbf{u} \operatorname{div}\dot{\mathbf{u}} + c^2 \operatorname{rot}\mathbf{u} \circ \operatorname{rot}\dot{\mathbf{u}}\,. \tag{23}$$

Using identities $\operatorname{div}(a\mathbf{u}) = \mathbf{u} \circ \operatorname{grad} a + a \operatorname{div}\operatorname{grad}\mathbf{u}$ and $\operatorname{div}(\mathbf{A}\times\mathbf{B}) = \mathbf{B} \circ \operatorname{rot}\mathbf{A} - \mathbf{A} \circ \operatorname{rot}\mathbf{B}$, the formula (23) becomes

$$\frac{\partial e}{\partial t} - \operatorname{div}\left[3c^2 \left(\operatorname{div}\mathbf{u}\right)\dot{\mathbf{u}} - c^2\left(\operatorname{rot}\mathbf{u}\right)\times\dot{\mathbf{u}}\right] = 0. \tag{24}$$

Comparing (21) and (24), the energy flux equals $S = c^2\left(\operatorname{rot}\mathbf{u}\right)\times\dot{\mathbf{u}} - 3c^2\left(\operatorname{div}\mathbf{u}\right)\dot{\mathbf{u}}$ or in the quaternionic notation

$$\hat{S} = c^2 \hat{\phi} \times \hat{\dot{\mathbf{u}}} - 3c^2 \sigma_0 \hat{\dot{\mathbf{u}}} \tag{25}$$

or equivalently

$$\hat{S} = c^2\left(\sigma - \sigma_0\right) \times \hat{\dot{\mathbf{u}}} - 3c^2 \sigma_0 \hat{\dot{\mathbf{u}}}\,. \tag{26}$$

Thus, the relation (21) can be written in the form of the continuity equation

$$\frac{\partial e}{\partial t} + \operatorname{div}\hat{S} = 0\,. \tag{27}$$

Moreover from (27) and the Gauss theorem we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} e\,\mathrm{d}\Omega = \int_{\Omega} \frac{\partial e}{\partial t}\,\mathrm{d}^3\mathbf{r} = -\int_{\Omega} \operatorname{div}\hat{S}\,\mathrm{d}^3\mathbf{r} = -\int_{\partial\Omega} \hat{S} \circ \hat{\mathbf{n}}\,\mathrm{d}\left(\partial\Omega\right), \tag{28}$$

where $\hat{\mathbf{n}}$ is a normal outside vector to the boundary $\partial\Omega$, $\hat{\mathbf{n}} = n_1\mathbf{i} + n_2\mathbf{j} + n_3\mathbf{k}$. Hence the condition

$$\int_{\partial\Omega} \hat{S} \circ \hat{\mathbf{n}}\,\mathrm{d}\left(\partial\Omega\right) = 0 \tag{29}$$

is equivalent to the law of energy conservation (20) and it is a well posed nonlocal boundary condition for Eqs. (11)-(15).

The Klein-Gordon equation fulfills the laws of special relativity, but contains two fundamental problems [12]. The first one is that it allows negative energies as a solution. As can be seen, the energy computed using formula (20) and solutions of Eq. (15) is per definition always positive. The second problem of the KGE is the indefinite probability density, e.g., it allows negative probabilities. From Eqs. (26) and (27) it follows that such a situation is avoided in the derived wave equation.

6. Conclusions

The alternative, mathematically correct derivation of the quaternion form of the momentum conservation law in an elastic solid is presented. Using the quaternion algebra, we demonstrated the transition from the classical Navier-Cauchy motion equation to its quaternion valued analogue. This quaternionic analogue elucidates the coupling between the irrotational and solenoidal displacement in the deformation field (compression and torsion) and allows for a physical interpretation of the wave mechanics and lets some of the quantum mysteries disappear. Below we compare the classical and quaternion forms of the equation of motion. The last column shows the terms that vanish in Eqs. (3) and (11) but contain information on the oscillation of internal energy due to the deformation caused by the spatially localized wave. These terms are essential to get system (12).

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} = c^2\left(2\Delta\mathbf{u} - 3\,\mathrm{rot}\,\mathrm{rot}\,\mathbf{u}\right) + c^2\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u} + \nabla V(t) - \nabla V(t), \left[\frac{\mathrm{m}}{\mathrm{s}^2}\right]$$

$$\begin{bmatrix}\text{momentum}\\ \text{change per}\\ \text{mass unit}\end{bmatrix} = \begin{bmatrix}\text{torsion \& compre-}\\ \text{ssion: "wave force"}\\ \text{per mass unit}\end{bmatrix} + \begin{bmatrix}\text{compression force}\\ \text{per mass unit}\end{bmatrix} + \begin{bmatrix}\text{gradient of mech-}\\ \text{anical potential}\\ \text{per mass unit}\end{bmatrix}$$

Quaternion analogue: $\Downarrow$

$$\frac{\partial^2 \sigma}{\partial t^2} = c^2\Delta\sigma + 2c^2\Delta\sigma_0 + \frac{8\pi m}{m_P t_P^2}\left(\sigma\cdot\sigma^* - \sigma\cdot\sigma^*\right), \left[\frac{1}{\mathrm{s}^2}\right]$$

$$\begin{bmatrix}\text{momentum change}\\ \text{per Planck}\\ \text{particle \& length}\end{bmatrix} = \begin{bmatrix}\text{torsion \& compression:}\\ \text{"wave force" per}\\ \text{Planck particle \& length}\end{bmatrix} + \begin{bmatrix}\text{compression force}\\ \text{per Planck}\\ \text{particle \& length}\end{bmatrix} + \begin{bmatrix}\text{fluctuation of mechani-}\\ \text{cal potential per Planck}\\ \text{particle \& length}\end{bmatrix}$$

We derived a spatially localized nonlinear wave function that is equivalent to the particle:

$$\partial_\mu \partial^\mu \sigma + 8\pi \frac{mc^2}{\hbar t_P}\sigma^* \sigma = 0$$

and its essential consequence, the formula for the irrotational potential field (gravity field):

$$\Delta\phi = 4\pi\rho G \text{, where } \phi = -c^2\sigma_0 .$$

The wave and Poisson equations were derived from assumptions which are independent of the postulates of quantum mechanics. The formulae for the local energy density in its quaternionic form allow obtaining the nonlocal boundary conditions providing the energy conservation. The energy computed using a new wave equation is per definition always positive. The problem of the indefinite probability of the density, present in classical KGE, is ruled out as well.

This derivation is new evidence that there is a well-defined mathematical connection between classical and quantum mechanics. The method allows the self-consistent classical interpretation of the wave phenomena and yields the non-relativistic gravity field. It is obvious that it can be generalized upon neglecting the assumptions of the constant density of mass and the constant Young modulus within the deformation field.

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Анотація. Данілевські М., Сапа Л. Нелінійне рівняння Клейна-Гордона у пружному твердому середовищі Коші-Нав'є. *Показано, що кватерніонна теорія поля може бути строго отримана з класичних рівнянь балансу в ізотропному ідеальному кристалі, де передавання імпульсу і енергія поля описуються рівнянням Коші-Нав'є. Теорія представлена у вигляді нелінійного хвильового рівняння та рівняння Пуасона з кватерніоно-значними хвильовими функціями. Отримана кватерніонна форма рівняння Коші-Нав'є зв'язує між собою стиснення і кручення поля зміщень. Хвильове рівняння має вигляд нелінійного рівняння Клейна-Гордона та описує просторово локалізовану* *хвильову функцію, еквівалентну частинці. Виведене рівняння хвилі уникає проблем негативної енергії та ймовірності. Дається самоузгоджена класична інтерпретація хвильових явищ та гравітації.*

Ключові слова: квантова хвиля, кватерніонна алгебра, рівняння Клейна-Гордона, гравітація.

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A. Gokhman, D. Terentyev, M. Kondria

ISOCHRONAL ANNEALING OF ELECTRON-IRRADIATED TUNGSTEN MODELLED BY CD METHOD: INFLUENCE OF CARBON ON THE FIRST AND SECOND STAGES OF RECOVERING

The evolution of the microstructure of tungsten under electron irradiation and post-irradiation annealing has been modelled using a multiscale approach based on Cluster Dynamics simulations. In these simulations, both self-interstitials atoms (SIA) and vacancies, carbon atoms isolated or in clusters, are considered. Isochronal annealing has been simulated in pure tungsten and tungsten with carbon, focusing on recovery stages I and II. The carbon atom, single SIA, single vacancy and vacancy clusters with sizes up to four are treated as the mobile pieces. Their diffusivities as well as the energy formation and binding energies are based on the experimental data and ab initio predictions and some of these parameters have been slightly adjusted, without modifying the interaction character, on isochronal annealing experimental data. The recovery peaks are globally well reproduced. These simulations allow interpreting the second recovery peak as the effect of carbon.

Key words: Post-irradiation Annealing**,** Tungsten, Carbon Effect, Cluster Dynamics.

1. Introduction

Tungsten is one of the candidate materials for the plasma facing component of fusion reactors because of its high melting point, high sputtering resistivity, and high temperature strength. Numerous studies have explored the recovery processes of radiation-induced damage in tungsten. Residual electrical resistivity was commonly used as an index of the damage present in materials for the damage recovery study, resulting in the identification of the temperatures and activation energies for different annealing stages. To date, the physical mechanisms governing the damage recovery of tungsten are still controversial. The next progress in study of this phenomenon could be done by Cluster Dynamics (CD) and Adaptive Kinetic Monte Carlo (AKMC) simulations. In our paper CD is applied to simulate the kinetics of point defects in post-irradiation annealing tungsten after electron irradiation. Special attention to effect of carbon is devoted.