THREE-PHASE POLYME NANOCOMPOSITE MATERIAL

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Abstract. Today, nano composite material is being studied and widely used for defence security and economic development. Keeping researching on the mechanic of three-phases nano composite in which two-phases is grains of pad and the structure of one-phase in reinforced two-phases is a nano structure, basing on consideration for interaction of the polyme matrix and grains of padding, we have defined engineering constants of the three-phases polyme composite nano material.

1. Nano material and its applications

The idea about super-small structures was raised by the American scientist Feynman R.P, a Nobel prize winner for physics, when he presented the students his lectures in 1959 and then these lectures were colected to build a book "There is plenty of room at the bottom in Minituarization. New York; Rienhold", published in 1960. In these lectures, he dealt with super-small structures and predicted that there would be new materials structured by graining size 10^{-7} -10^{-9} metre.

Since 1970, only 11 years after the birth of the idea about nano structure, USSR, USA, Japan.v.v... have carried out the process of building nano technology simultaneously with transistorized material.

However, not until 1981 did the Denmark scientist Gleiter H. officially bring up a question for new nano structured material and immediately it drew a special attention from the USA, the USSR, Japan and China. In 1983, the Russian scientist Iakovlev E.N. announced his first work on producing Niken structured by nano which was made of micro structures.

Nano technology is applied throughly in manufacturing Medical Tools [2,9] such as: micro engines implanted in choked up vessel for carrying out on-the-spot emergency, circulating blood or taking drugs to the needed cells of the body; micro-equipment taking drugs and chemicals implanted in cancer tissues to destroy cancer cells. Nano technology also helps to identify accurately and quickly genecode, facilitating the predicting, diagnosing and treating of diseases,...

Nano material is also widely used in industry [3,4,5,8,12] when changing the structure of Graphite as replacing an atom of carbon in Graphite crystal system with one metal (like bronze) we can get transsitorized carbon. Bronze nano material can get rid of vibration effectively, twice to three times better than grey cast iron, a material up to now has been considered as one which has an ideal ability of anti-vibration. Zicondioxide nano pottery owns many more good points, burning at 1250°C, while normal porttery burning at 1600°C, so producing nano pottery we not only receive a new better material but also reduce noticeably energy resource needed for the producing process. Metal materials plated with nano seeds can increase the hardness from 16 to 63% depending on the type of seed, the thickness of the plating and fines of seeds. Instead of cumbersome mine-detector, nowadays America has begun applying nano technology to manufacture 7.5 cm-diameter mine-inspector robots. Owing to applying nano technology, microchips with very large memory and super speed computers have been produced. It is estimated that we can creat information stores of one gram eath but with the memory as large as a national library. Nano materials, undoubltedly are likely to make something incredible in the 21^{st} century and their products will come out of laboratories establishing a real industrial revolution.

There are 3 main orientations in researching on nano technology field in the world:

- Basic research (calculating, building models, studying phenomena…)
- Manufacturing technology
- Applying nano technology, applying methods, exploiting effectively.

The governments of developed countries have paid much attention to nano technology and considered it as one of the priorities in development orientations. Today, Western Europe is a leading region in researching and applying nano technology [4,8]. In order to catch up with information and achievements of other countries, America must adjust policies and investments to strengthen the relationships with other nations, exchange information, carry out joint researches and train young scientists in this field. Up to now, America has owned over 20 large scale programs, projects and 22 universities have the ability of educating students studying applying nano technology [8].

With the information we have now, besides America and Russia, it is estimated that there will be large leading centres of nano technology in Japan, China, France, Germany, Israel, Finland and South Korea,…

Scientists affirm that nano technology will create a great effect on our social life: thanks to nano technology, goods will be more durable, more qualified and because of using new materials health care service will be more effective, popular and cheaper; there will be new drugs, new medical tools as well as man-made body organs. Nano technology will also change the education system to update more adequately and all sidedly the knowledge of this high technology. With the birth of nano technology, there will be new type of energy which helps to maintain unpolluted enviroment, even new kind of foods that unprecedentedly appear in any menu. Nano technology will change the working conditions, travelling and services. The average human age will consequently increase in the 21^{st} century. Many Scientists have agreed that the discoveries of the steam engine, the electricity, lazer and nano technology have up to now been the most important ones in human society.

The development in researching and applying nano technology not only brings human beings back the fresh knowledge and discoveries of the wild world, but also motivates strongly the global economy. If applying nano technology brought about a revenue of 45 billion US dollar in 2001, it is estimated that only in 10 or 15 years, the revenues brought about by nano technology will mount up to more than 1000 billion US dollar in which:

- 340 billion earned from new materials
- 300 billion from transistorized industry
- 180 billion from pharmacy and medical tools
- 100 billion from industrial chemicals and catalyst
- 70 billion from transportation
- 100 billion from environment and natural resources protection.

Expressing in the semina named “The social impacts of the nano science and technology”, in America in September 2000, scientists agreed that in 15 to 20 years, nano technology will change basically science, technique and society. They simultaneously warned the danger of threatening human being as nano technology will cause great effect on information, biology, health care and defence fields. Scientists also realized that: Today, nano technology is on its first steps of development, because what people have achieved is much smaller than the extremely great potentiality nano technology could bring back.

2. Model of the three-phase polyme nanocomposite material

To have a unified concept, in many references the structures which are smaller than 100 nano metre are considered as nano structures.

Today, there are 2 ways to create nano structure. The first one is “From bigger to smaller”, for example people “grind” the bigger structure until they get the expected smaller ones. The second is “Turn one into another”, which means changing the inside order of the atoms or the molecules, changing the order of seeds to make new materials.

In Vietnam, some scientific articles on transitorized nano and magnetic materials have been issued recently. The issued documents about nano materials in our country now, however all follow the first way of creating nano structure “From bigger to smaller”, that means receiving nano structures from the bigger structures.

Composite is a material formed from 2 or more different materials in order to create new materials with more preeminent features than those of the original materials. Nano composite is the composite which has at least one of the elements forming nano structure.

In the researches before, we built a model of two-phase composite nano with polyme matrix and reinforced seeds which are nano. The initial results were that we determined the constants of the material. For instance, in fact when we use nanometre-size mineral and then mix with polyme to create composite which has some special characteristics such as: highly mechanical, heat - proof ability, anti-absorbent.

To boost the ability of mechanics and fire proof of polyme matrix when producing polyme, especially plastics, we use three-phase polyme: mixing a noticeble ratio of glass-seeds or carbon seeds, metallic seeds (to reinforce the ability of mechanic) and a small ratio of nano mineral seeds, nano clay seeds (to fireproof materials) into the polyme matrix. Nano composite nylon with 2 to 6% of nano clay seeds will be deformed at 150°C, meanwhile normal nylon will be melt at 60°C [8,9].

The model of the three-phase composite in this paper, therefore, include: polyme matrix, reinforced pad seeds and nano seeds (Fig 1)

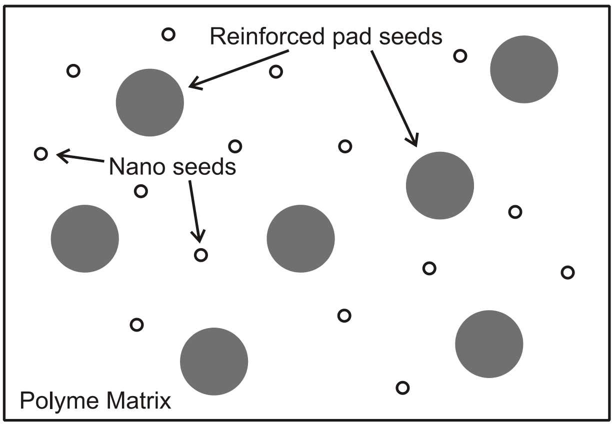

Fig 1. Model of the three-phase composite

We approach the nano structure according to method: "From bigger to smaller". Thus when researching the interaction of seeds with matrix we use the method of Newton mechanics [7,10,11,12]. The setting of the machanics problem of composite materials having sphere pad seeds and including interaction between pad seeds and matrix is built and calculated according to the model and method which were presented in [6,7,12].

3. Definition of constants of the material

For definition of constants of the composite material (fig 1), we suppose that reinforced seeds which have the same radius a and super-small nano seeds have the same radius b. The component materials are isotropic, homogeneous and elastic.

From this supposition, the three-phase composite problem will be solved according to two-phase model with algorithm as follows: at first, the constants of the two-phase composite material which includes polyme matrix and reinforced seeds are defined (problem A), as a result we receive a isotropic, homogeneous and elastic material. This material will be counted as a matrix material for composite material in problem B and will be called supposed matrix material. At last, we deal with problem B of nanocomposite polyme, with supposed matrix material in which the constants of the material have been defined and pad nano seeds, taking their interaction into consideration.

The boundary problem of the elastic theory (problem A and B) have been built with displacement which satisfied the Lame equations

$$2(1-\nu)\text{grad} \quad \text{div} \quad \vec{u}-(1-2\nu)\text{rot} \quad \text{rot} \quad \vec{u}=0 \tag{1}$$

For micro stress problem in the near seeds being studied, we use local sphere coordinate with coordinate origin coinciding with the centre of seeds

$$x_1 = r \quad \cos \quad \theta, \qquad x_2 + ix_3 = r\sin\theta^{i\varphi} \tag{2}$$

The condition on the boundary of contact between seeds and polyme matrix is built as follows (r = a)

$$\begin{gathered} \sigma_r^+ = \sigma_r^-, \sigma_{r\theta}^+ = \sigma_{r\theta}^-, \sigma_{r\varphi}^+ = \sigma_{r\varphi}^+ \\ u_r^+ = u_r^-, u_{r\theta}^+ = u_{r\theta}^-, u_{\varphi r}^+ = u_{\varphi r}^- \end{gathered} \tag{3}$$

In the tension - compress case, the stress of the mechanic problem satisfied the equilibrium equation

$$\sigma_{ij,\ j} = 0 \tag{4}$$

Micro – stress in matrix – material is defined by

$$\begin{aligned} \sigma_r &= R + 4G\frac{M}{r^3} + 2G\left(\frac{Q}{G} - \frac{20-4\nu}{r^3}N + \frac{12}{r^5}F\right)P_2(\theta) \\ \sigma_{r\theta} &= 2G\left(\frac{Q}{2G} - \frac{2(1-\nu)}{r^3}N + \frac{4}{r^5}\right)\frac{dP_2(\theta)}{d\theta} \end{aligned} \tag{5}$$

Strain in matrix material is defined by

$$\begin{aligned} u_r &= \frac{R}{3K}r - \frac{M}{r^2} + \left(\frac{Q}{G}r + \frac{10-8\nu}{r^2}N - \frac{3F}{r^4}\right)P_2(\theta) \\ u_\theta &= \left(\frac{Q}{2G}r + \frac{2-4\nu}{r^2}N + \frac{F}{r^4}\right)\frac{dP_2(\theta)}{d\theta} \end{aligned} \tag{6}$$

in which

$$P_2(\theta) = \frac{1}{2}\left(3\cos^2\theta - 1\right), \qquad K = \frac{E}{3(1-2\nu)}$$

$$R = \frac{1}{3}\left(\sigma_1^0 + \sigma_2^0 + \sigma_3^0\right), \quad Q = \frac{1}{6}\left(2\sigma_1^0 - \sigma_2^0 - \sigma_3^0\right)$$

Micro stress impacting in pad seeds is in the form of

$$\begin{aligned} \sigma_{rc} &= 2G\left\{-2(1+\nu_c)A_0 + \frac{2D_0}{r^3} + \left[-6\nu_c A r^2 + 2B - 4(5-\nu_c)\frac{C}{r^3} + \frac{12D}{r^5}\right]P_2(\theta)\right\} \\ \sigma_{r\theta c} &= 2G_c\left[(7+2\nu_c)Ar^2 + B + 2(1+\nu_c)\frac{C}{r^3} - \frac{4D}{r^5}\right]\frac{dP_2(\theta)}{d(\theta)} \end{aligned} \tag{7}$$

According to the calculating results of Kristensen basing on Esenpi principle [1], the result of problem A is a composite which has 2 elastic constants and is defined follows

$$\frac{\bar{G}}{G} = 1 - \frac{15(1-\nu)\left(1-\frac{G_1}{G}\right)\xi_1}{7-5\nu+2(4-5\nu)\left(\frac{G_1}{G}\right)}, \qquad \bar{K} = K + \frac{(K_1-K)\xi_1}{1+(K_1-K)\left(K+\frac{4}{3}G\right)^{-1}} \tag{8}$$

In this paper, the values are symbolised with low-subscript "c" that denotes pad sphere seeds; low-subscript "1" denotes reinforced seeds; low-subscript "2" denotes nano seeds and non-subscript denotes real polyme matrix; overbar "-" denotes supposed matrix; circumflex accent "^" denotes constants of the three-phase nanocomposite which need to be found. ξ_1, ξ_2 are the ratio of the distributed volume of the nano and reinforced seeds in the composite, respectively.

For problem B: micro-stress in the composite material is defined as follows

$$\sigma_{ik} = \sigma_{ik}^0 + \sigma_{ik}^* + \sigma_{ik}^{**} + \ldots \tag{9}$$

where:

σ_{ik}^0 homogeneous stress

σ_{ik}^* reciprocal stress between matrix and seeds

σ_{ik}^{**} reciprocal stress between the nearest seeds

In this paper, we only research on reciprocal stress between matrix and seeds, which means considering the first and second terms in expression (9).

Using our results in [6,7,12], we receive a composite material, which is isotropic, homogeneous and elastic and it has 2 elastic constants. The final result is defined as follows

$$\hat{K} = \bar{K}\frac{\left(K_2+\frac{4}{3}\bar{G}\right)+4\xi_2\bar{G}\left(K_2-\bar{K}\right)\left(3\bar{K}\right)^{-1}}{\left(K_2+\frac{4}{3}\bar{G}\right)-\xi_2\left(K_2-\bar{K}\right)}$$

$$\hat{G} = \frac{1-\xi_2(7-5\bar{\nu})\left(\frac{\bar{G}}{G_2}-1\right)\left[8-10\bar{\nu}+(7-5\bar{\nu})\frac{\bar{G}}{G_2}\right]^{-1}}{1+\xi_2(8-10\bar{\nu})\left(\frac{\bar{G}}{G_2}-1\right)\left[8-10\bar{\nu}+(7-5\bar{\nu})\frac{\bar{G}}{G_2}\right]^{-1}} \tag{10}$$

For receiving formula to defining the constants of nano composite polyme material according to the constants of components of the initial three-phase material, we only replace elastic modules of the supposed matrix material (8) into formula (10).

To illustrate, we consider two-phase composite, which has epoxy matrix – Boric metallic seeds with $\xi_1 = 0.3$ (straight line in Fig 2, which is calculated according to Kristensen for Boric-Epoxy two-phase composite), and epoxy matrix three-phase composite with basaltic mineral nano seeds and Boric metallic seeds with $\xi_1=0.3$, $\xi_2=0.1$ (expressed by curved line in Fig 2, which is my calculated result for three-phase composite, considering the interaction between nano seeds and the supposed matrix).

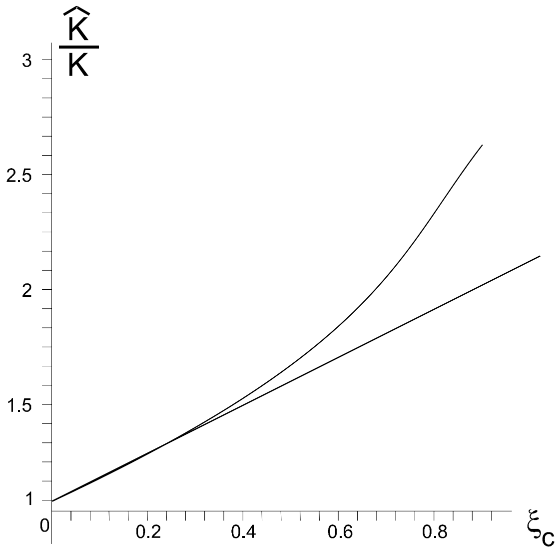

Fig 2. Calculated result for Moduli K of the two-phases and three-phases composite

From the results we have received, we realize that elastic modules of material will raise if we add nano seeds into polyme matrix material.

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References:

1. Christensen R.M. Mechanics of composite materials. University of california, New York, 1979.
2. Lee S.C. The nanobiological strategy for constructions of nanodevices. In Lee S.C. and L. Savage(eds), *Biological molecules in nanotechnology: the convergence of biotechnology, polymer chemistry and materials science*. Southborough, MA: IBC Press. 1998.
3. Tilden M.V. Autonomous biomorphic robots as plaforms for sensors. report Number LA-UR -96-3222, U.S. Information Bridge , DOE Office of Scientific and Technical Information(OSTI),1998.

4. Meyer M. and Persson O. Nanotechnology - interdisciplinarity, patterns of collaboration and differences in applications. *Scientometrics 42(2)*, 195, 1998
5. Lowe T.C., Bishop A., Burns C.,...Nanoscale science and technology at Los Alamos national laboratory. *J.Nanoparticle Research 2*, 249, 2000
6. Nguyen Dinh Duc. "Mechanics of nano-composite material" .*J. of science of Vietnam national University, Hanoi : Mathematics-physics*, T.XIX, N4, 2003.
7. Нгуен Динь Дык.*Сферfinancial волокнистые композиты с пространственной структурой*. Москва "УРСС", 2000, 242 с.
8. *Нанотехнология в ближайем десятилетии*: Прогноз направления исследования. Под редакцией М. К. Роко и другие. Москва "Мир", 2002
9. Помогайло А.Д., Розенберг Ф.С., Уфлянд И.Е. *Наночастицы металов в полимерах* . Москва, "Химия", 2000
10. Nguyen Hoa Thinh, Nguyen Dinh Duc. *Composite Materials: Mechanics and Technology*. Science and Technical Publisher, Hanoi, 2002.
11. Dao Huy Bich, Nguyen Dang Bich. *Continuous medium Mechanics.* Hanoi National University Publisher, Hanoi, 2003.
12. Nguyen Dinh Duc. *Mechanics of Polyme Nanocomposite Material*. Scientific Report at the7th National Conference on Mechanics of deformed solid. Doson, 27-28/7/2004.