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QUANTITATIVE DESCRIPTION OF THE MIXING OF METALS UNDER SEVERE PLASTIC DEFORMATION

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Abstract. Solid-phase synthesis by joint plastic deformation of the components under high pressure opens up completely new possibilities in creating new materials. A key step in the materials synthesis during severe plastic deformation (SPD) is the delivery of atoms of different components to specific locations in the sample. It is carried out due to the mixing process in the solid phase. The details of the process are still largely unexplained in microstructural terms. This hinders the employment of the enormous potential of SPD synthesis.

The report presents the results of studies on a mixing of metals during the formation of nanostructured metal compositions by SPD technique.

<u>Keywords</u>: solid-phase synthesis; severe plastic deformation; high pressure torsion; copper; aluminum; layers; mixing

When creating new materials, the starting components are combined with each other, usually in a liquid state. Solid-phase synthesis by joint plastic deformation of the components under high pressure opens up completely new possibilities in this regard. The guiding principle was proposed by the Nobel Prize winner Percy Williams Bridgman. He suggested an innovative technique based on the torsion of samples in the form of thin disks between two anvils, and used it to create alloys and polymers in his first experiments [1, 2]. The sample was compressed between the anvils during the deformation under an applied pressure of tens of thousands of bars. Today the technique is known as High Pressure Torsion (HPT).

Since the late 1980's, HPT has been widely used to create ultrafine-grained metals and alloys with remarkable physical and mechanical characteristics [3]. In addition to HPT other techniques were developed, based on the Bridgman's idea to stimulate phase transformation by applying large deformations. This approach has a common name of SPD [4].

A key step in the materials synthesis during SPD is the delivery of atoms of different components to specific locations in the sample. It is carried out due to the mixing process in the solid phase. One can distinguish the mixing at different spatial scales. We can outline the synthesis during the SPD as follows. The starting material has rather large structural characteristic size of tens or hundreds of micrometers and can be used in various shapes, such as wires, tapes, plates, powder particles, etc. During SPD, they are thinned to micron and submicron scale, fragmented into small pieces and mixed together. In parallel, crystal lattice defects including vacancies, dislocations, and grain boundaries are formed, leading to the mechanical activation of the material and acceleration of the diffusion processes. High hydrostatic pressure in the deformation zone prevents the failure of the material. All this creates the conditions for the formation of solid solutions, new phases, and chemical compounds, even those that cannot be obtained by liquid-phase approach.

The scheme of SPD synthesis looks rather understandable and was already presented by P. Bridgman in his first works [1, 2]. However, the details of the process are still largely unexplained in microstructural terms. This hinders the employment of the enormous potential of SPD synthesis, since without the knowledge of the process details it is impossible to gain the desired result. In particular, without understanding the mechanisms of solid-phase mixing, it is not possible to ensure the necessary distribution of substances throughout the sample volume.

In order to quantitatively study the mixing process, a parameter characterizing the degree of mixing is introduced in the work. This is done as follows. Let us consider schematically the process

of mixing two substances, A and B. They are completely separated in the initial state, and their volume fractions are equal to a and b respectively (a + b = 1) (Fig. 1).



Fig.1. Scheme of mixing two components (a – initial, b – after deformation)

During the mixing, regions with two substances are formed (Fig. 1b). We define a parameter that would characterize the degree of mixing of substances in such areas. In the study of mixing, first of all, it is necessary to determine the size of the averaging area, which allows introducing such concepts as the concentration of components and field characteristics of mixing. This area plays the role of a representative volume in the mechanics of continuous media. Its characteristic size should be determined by the physics of the process. In the study of mixing, the averaging area will be considered a point, similar to material points in the mechanics of continuous media.

We will consider only two scale levels, each of which is associated with its determinative mechanisms of mixing. For the lower scale level, where mixing is due to diffusion, the characteristic sizes satisfy the condition $l < l_d$, where l_d is the characteristic size of the diffusion zone ($l_d = \sqrt{2D_{eff}\tau}$, where τ is the characteristic diffusion time and D_{eff} is the effective diffusion coefficient). According to preliminary estimations $l_d \sim 1 \ \mu m$.

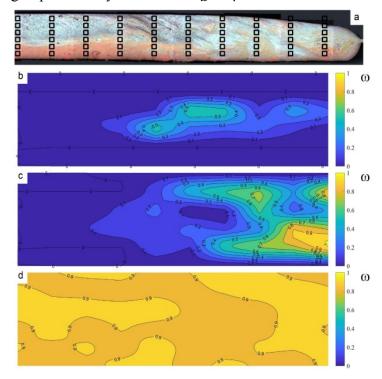


Fig. 2. Scheme of the ω index distribution through the sample cross section (a – scheme of samples with points of XRD analysis, b, c, d – distribution of ω index for beginning, middle and complete intermixed stages two layers respectively)

The upper scale level is characterized by the lengths $l_d \ll l < L$, where L is the size of the sample (the area that the components originally occupy). At this level, mixing is due to the mechanisms of advection mass transfer. Studies of mixing at the upper and lower scale levels will be performed according to their respective methods. Below we describe the technique proposed for the mixing at the upper scale level. At the upper level, we introduce the concepts of concentration

of components $\xi_a(\mathbf{r})$ and $\xi_b(\mathbf{r})$, by which we mean the volume fractions of components A and B in the averaging zone, centered at a point \mathbf{r} . Obviously, $\xi_a(\mathbf{r}) + \xi_a(\mathbf{r}) = 1$. The numbers $\xi_a(\mathbf{r})$ and $\xi_b(\mathbf{r})$ are determined by EDX analysis, with a spot size $\sim l_d$. As a measure of mixing $\omega(\mathbf{r})$, we take a value that satisfies the following conditions:

- (1) in areas where there is no mixing, when $\xi_a = 0$ and $\xi_a = 1$, $\omega = 0$;
- (2) for perfect mixing, when $\xi_a = a$, the value ω reaches a maximum of 1.

A variety of expressions can satisfy these conditions, of which we take the simplest:

$$\omega = \begin{cases} \frac{\xi_a}{a}, & when \ \xi_a \le a \\ \frac{1 - \xi_a}{1 - a}, & when \ \xi_a > a \end{cases}$$

As an example, Fig. 2 shows the distribution of the ω value for the workpiece of two layers of copper and aluminum of equal thickness under the HPT deformation.

The aim of the experiment was to restore the $\omega(r)$ field in the sample volume according to the results of its measurements in various sections of the sample. In the experiment, we have studied the dependency of $\omega(r)$ on the properties of the materials, the geometric characteristics of the initial sample, the number of the anvil rotations, and the deformation temperature.

Кількісний опис змішання металів при інтенсивній пластичній деформації Бейгельзімер Я.Ю., Кулагін Р.Ю., Давиденко О.А., Дмитренко В.Ю.

Твердофазний синтез шляхом спільної пластичної деформації компонентів під високим тиском відкриває абсолютно нові можливості в створенні нових матеріалів. Ключовим етапом синтезу матеріалів під час інтенсивної пластичної деформації (ППД) є доставка атомів різних компонентів в певні місця в зразку. Це здійснюється за рахунок процесу перемішування в твердій фазі. Деталі процесу все ще значною мірою не пояснені з точки зору мікроструктури. Це перешкоджає використанню величезного потенціалу ППД-синтезу. У доповіді представлені результати досліджень змішування металів при формуванні наноструктурованих металевих композицій методом ІПД.

Ключові слова: твердофазний синтез; інтенсивна пластична деформація; крутіння під високим тиском; мідь; алюміній; шари; змішування.

Количественное описание смешения металлов при интенсивной пластической деформации

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Твердофазный синтез путем совместной пластической деформации компонентов под высоким давлением открывает совершенно новые возможности в создании новых материалов. Ключевым этапом синтеза материалов во время интенсивной пластической деформации (ИПД) является доставка атомов различных компонентов в определенные места в образце. Это осуществляется за счет процесса перемешивания в твердой фазе. Детали процесса все еще в значительной степени не объяснены с точки зрения микроструктуры. Это препятствует использованию огромного потенциала ИПД синтеза.

В докладе представлены результаты исследований смешения металлов при формировании наноструктурированных металлических композиций методом ИПД.

Ключевые слова: твердофазный синтез; интенсивная пластическая деформация; кручение под высоким давлением; медь; алюминий; слои; перемешивание.

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