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Mechanism of Diffusion-Zone Formation at the Al–Fe Phase Interface under Impact-Loading Conditions

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A molecular dynamics study in combination with experimental research is applied for investigation of diffusion-zone formation on the phase interface between aluminium-based alloy Д16 (2024) and Fe-alloyed layer on its surface formed in the process of ultrasonic impact treatment (UIT) of Д16 alloy by Armco-iron pin. The formation of surface-layer structure, its thickening and diffusion zone formation between base material and alloyed layer is studied by scanning electron microscopy and energy-dispersive x-ray spectroscopic analysis of cross-section of treated samples. In the UIT process, the microstructure in the surface layer becomes finely fragmented and the diffusion zone becomes thicker with increasing of UIT duration. The molecular dynamics simulation is applied to investigate atom behaviour on the phase interface between Al- and Fe-layers, to observe defect formation and its migration in the process of impact loading, which contributes to the formation of diffusion zone and restructuring of near-phase interface layers.

Key words: impact treatment, dislocations, molecular dynamics, diffusion-zone, alloying, surface structure.

За допомогою методи молекулярної динаміки та експериментальної мето-

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дики з використанням ультразвукового ударного оброблення алюмінійового стопу Д16 бойком із армко-заліза досліджено механізми утворення дифузійної зони на межі поділу між матеріялом-основою та леґованим шаром, утвореним внаслідок оброблення. Формування структури поверхневого шару, зміну його товщини було досліджено за допомогою сканувального електронного мікроскопу. Також проведено хемічну мікрорентґеноспектральну аналізу поперечного перерізу оброблених зразків для дослідження товщини дифузійної зони між матеріялом основи та леґованим шаром. Встановлено, що в процесі ультразвукового ударного оброблення стопу Д16 бойком із армко-заліза товщина леґованого шару зростає, а його мікроструктура подрібнюється зі збільшенням тривалости оброблення. Товщина утвореної дифузійної зони на межі поділу між матеріялом-основою та леґованим шаром також зростає. Методою молекулярної динаміки досліджено поведінку атомів на межі поділу Al–Fe у процесі ударного навантаження та встановлено, що наявність межі поділу сприяє дефектоутворенню та взаємній міґрації атомів у такій системі, що приводить до формування дифузійної зони та зміни структури в прилеглих до межі поділу шарах.

Ключові слова: ударне оброблення, дислокації, молекулярна динаміка, дифузійна зона, леґування, поверхнева структура.

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1. INTRODUCTION

Depending on required properties, most metals and metal composites undergo thermal or mechanical treatments before exploitation. Thermal treatment mostly provides close to homogeneous microstructure of materials because of completed diffusion processes. Mechanical treatment mainly leads to strain hardening of materials. The significant property of constructive materials is surface hardness obtained by surface alloying with the following mechanical treatment. One useful example of such procedure is ultrasonic impact treatment (UIT) of aluminium-based alloy by the iron pin [1–3]. As shown, the surface alloying takes place by iron cladding on the aluminium-based specimen in the process of ultrasonic impact loading [4]. Impact treatment provides defect formation and atom migration on the phase interface and those atom-transfer processes are mechanically activated, as mechanical activated diffusion described in [5–7].

The main aim of this work is to study how does the mechanical alloying by UIT with Armco-iron pin contributes to the formation of diffusion zone on the phase interface between aluminium-based alloy Д16 and alloyed by Fe layer and what processes underlie it.

This work aims to reveal the contribution of the mechanical alloying by UIT with Armco-iron pin to the formation of diffusion zone on the phase interface between aluminium-based alloy Д16 and alloyed by Fe layer. The underlying processes are particularly addressed.

2. MATERIALS AND METHODS

Two samples of an aluminium-based alloy Д16 were treated using UIT by Armco-Fe pin in air conditions. The amplitude of the ultrasonic transducer was 25 μm, the treatment times were 90 s and 180 s. Treated samples were studied by the scanning electron microscope (SEM) Tescan Vega 3 to find out changings of near-surface microstructure and the thickness of alloyed layer. Energy-dispersive x-ray spectroscopic (EDS) analysis of cross-sections for both samples were done by EDS microanalyser OXFORD X-MAX 50 mm^2 to study out the thickness of the diffusion zone on the phase interfaces. SEM parameters were as follow: high voltage (HV) was 20 kV, magnification (Mag) was 10000, beam intensity (BI) was 13, working distance (WD) was 15 nm, accelerating current (AC) was 450 pA, spot size (SS) for EDS chemical analysis was 180 nm.

Another part of research was a molecular dynamics study of the interface region between f.c.c. Al and b.c.c. Fe under impact loading for better understanding of defect occurring and mass-transfer processes in near-surface layers under UIT. The model was built using modified embedded-atom method for describing interatomic interactions [8]. The modelled samples consisted of a big layer of Al (18.6 nm in X direction, 22.2 nm in Y direction and 3.1 nm in Z direction) and a layer of Fe with the same dimensions in X and Z directions and different thickness (7 nm, 21 nm, 63 nm) in Y direction in order to sample. The impact loading was realized by displacing of fixed atom layer on the surface of modelled sample in the only X direction. Another two directions (Y and Z) were built with the periodic boundary conditions. The molecular dynamics models were studied at temperature 300 K with previous slow heating of the modelled samples from 0 K to 300 K and next atom displacing. The equilibrium lattice parameters at 0 K and 300 K for Al and Fe, modelled using potential [8], were calculated (Table 1) by establishing zero stresses in a calculating cell.

Given deformation rate, contributing by atom displacing, in modelled samples was of 13 m/s that is close to the deformation rate under UIT. Full modelling time, including heating and atom displacing was of 66 ps, modelling time step was of 0.003 ps.

Images of modelled samples and some analysis of dislocations were

TABLE 1. Al and Fe equilibrium lattice parameters at different temperatures.

Temperature, K	Lattice parameter a, Å	
	Al	Fe
0	4.0335	2.8553
300	4.0377 (4.04 [9])	2.8572 (2.86 [9])

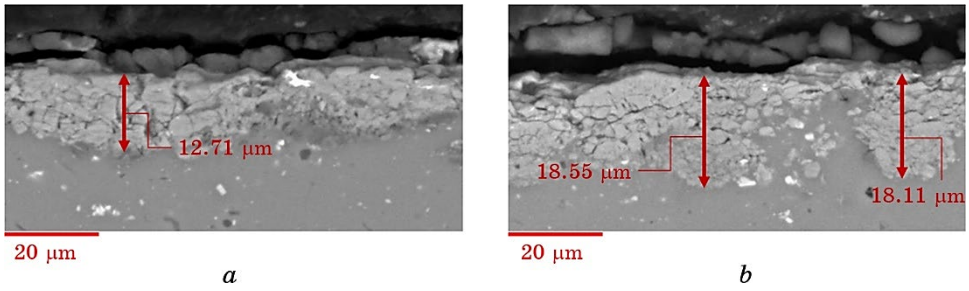

Fig. 1. The under-layer structure and the thickness of alloyed layer in Д16 alloy after ultrasonic impact treatment by Armco-iron pin during: 90 s (*a*), 180 s (*b*).

made with the help of OVITO package [10].

3. RESULTS AND DISCUSSION

In the process of UIT, the surface layer of Д16 alloy cowers by iron layer, forming a Fe-alloyed layer of Al, and following impact-loading leads to the Fe-alloyed layer thickening. According to SEM data, the thicknesses of alloyed layers are as follow: 12.7 μm after 90 s of treatment and 18.1–18.5 μm after 180 s of treatment (Fig. 1).

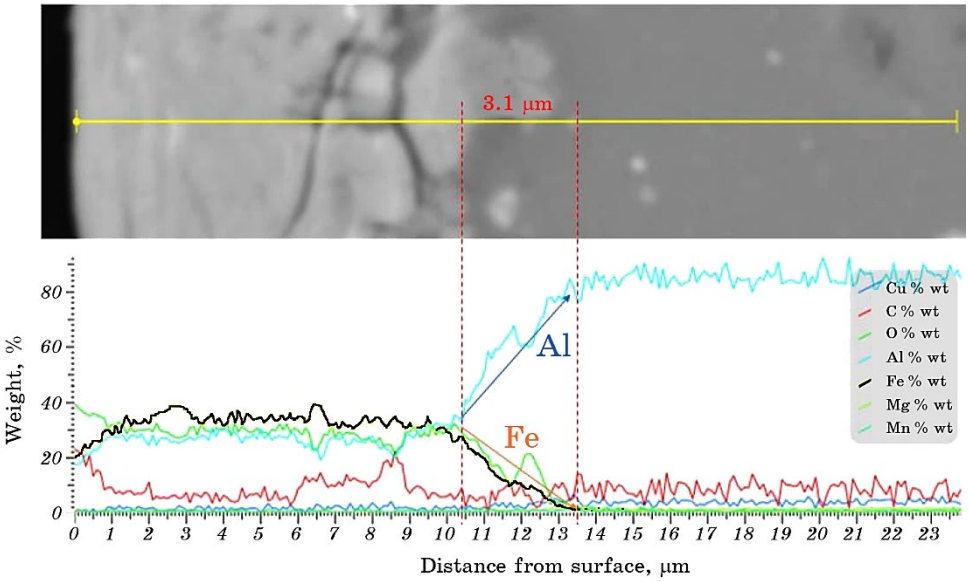

Fig. 2. The formation of diffusion zone in Д16 alloy after ultrasonic impact treatment by Armco-iron pin during 90 s.

In addition to thickening of alloyed layer with the duration of UIT, the surface structure becomes more dispersive, as can be seen from the comparison between Fig. 1, *a* and *b*. It may be caused by defect formation and its migration in near surface layers in the process of impact loading.

Chemical analysis of cross section of Д16 alloy after Armco-iron pin UIT shows the formation of diffusion zone under alloyed layer near surface of specimen (Fig. 2, 3). The diffusion zone provides better adhesion between alloyed layer and base material.

As can be seen from the concentration profiles, the thickness of the diffusion zone after 90 s of UIT is 3.1 μm (Fig. 2), the thickness of the diffusion zone after 180 s of UIT is 4.6 μm (Fig. 3). In some cases, where the near-surface layer is more dispersed after 180 s of impact treatment, the diffusion zone thickness increases up to 7.5 μm.

A near-surface layer is not homogeneous and Fe forms segregations in the near-surface volume of aluminium alloy. Moreover, a small amount of Al segregates closely to the surface in the Fe-alloyed layer. The grain structure of alloyed layer crashes and grain size decreases with treatment continuance.

For better understanding of occurring on the phase interface processes and processes that lead to the formation of diffusion zone a molecular dynamics study has been applied.

At the beginning of modelling, f.c.c. structured Al atoms on the

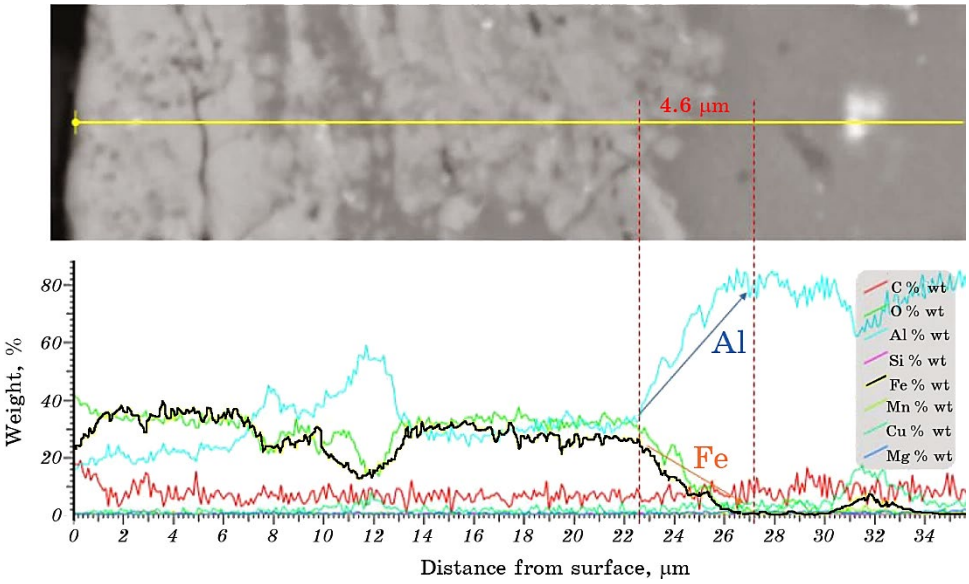

Fig. 3. The formation of diffusion zone in Д16 alloy after ultrasonic impact treatment by Armco-iron pin during 180 s.

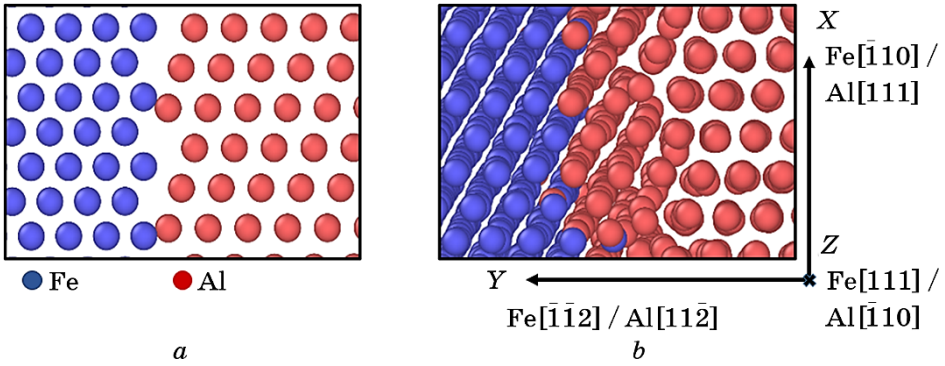

Fig. 4. A rebuilding of f.c.c. Al structure into b.c.c. on the phase interface Al–Fe (a part of modelled sample): initial lattice (*a*), after relaxation (*b*).

phase interface Al–Fe reconstructs into b.c.c. structured (Fig. 4) in the process of heating for three modelled samples with the different Fe-layer thickness.

Such Al structure transformation on the phase interface occurs because of more weight and higher binding energy of Fe atoms than Al atoms (that is why Fe atoms attract the nearest Al atoms to themselves). Besides, difference in lattice structures leads to the formation of a big amount of crystal defects. The subsequent impact treatment is a reason for the formation of point defects (mainly interstitial atoms) and glide dislocations. As the study of the structure in the process of modelling shows, the phase interface is a source of dislocation for-

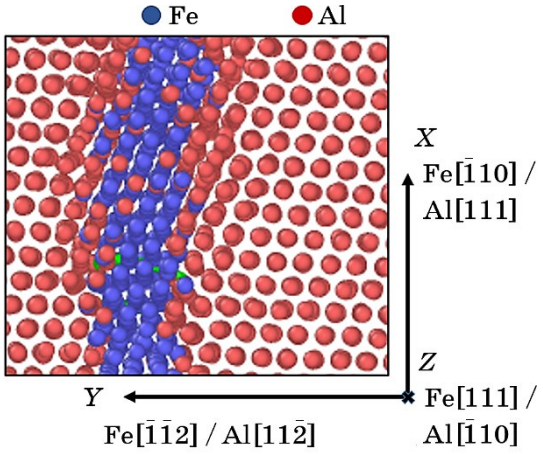

Fig. 5. Atom migration on the phase interface Al–Fe in a sample with 7 nm Fe layer (a part of modelled sample). Green lines are dislocation lines.

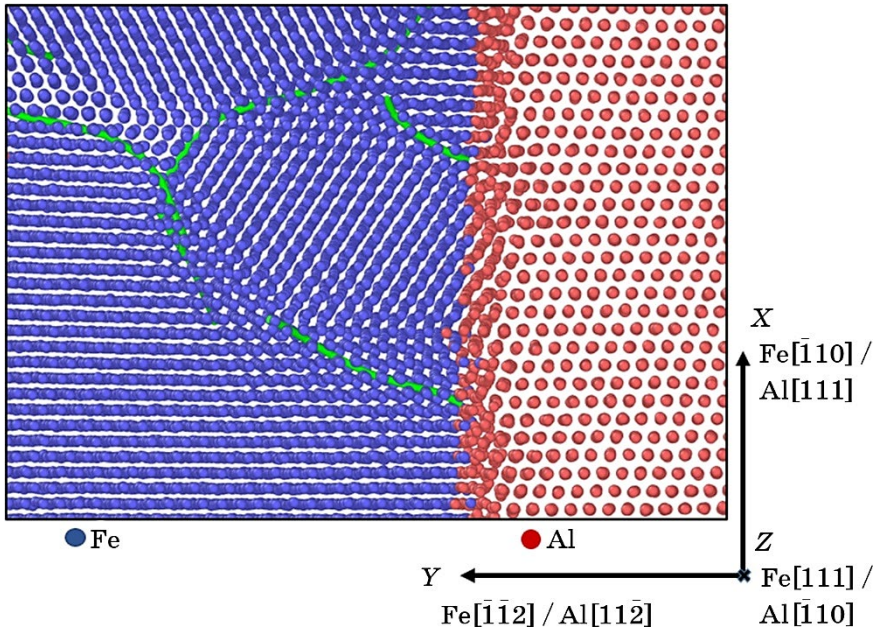

Fig. 6. Restructuring of Fe layer in the process of impact loading modelling (a part of modelled sample). Green lines are dislocation lines.

mation in both materials. During the heating and deformation, Shockley dislocations (Burger's vector $b = (a/6)\langle 112\rangle$) appear a lot in Al near the phase interface with Fe layer. Dislocations with Burgers vector $b = (a/2)\langle 110\rangle$ appear in Al layer only in a process of crystal deformation.

In a sample with thin Fe layer (7 nm), where stresses in Fe volume are the highest, a big amount of dislocations ($b = (a/2)\langle 111\rangle$) in Fe appear during heating, what is not observed for samples with Fe layers 21 nm and 63 nm, where first dislocations appear only after beginning of deformation. Such behaviour of sample with the thinnest Fe layer can be described by a significant contribution of face interface stresses like the influence of surface in nanostructured materials, which leads to the deformation of surface shape and to changings of thermal properties of those materials [11, 12].

Moreover, plastic deformation in modelled samples promotes the mutual migration of atoms on the phase interfaces. Defects, especially dislocations, occurring on phase interfaces, help to transfer diffused (interstitial) atoms into the volume of material in the way described in [5, 6].

There was observed that the mutual atom migration on the phase interface is more active in a case of the thinnest Fe layer (Fig. 5), because

the thickness of that layer is not enough for the phase interface stress relaxation in its volume and a large amount of compression and tension zones, in addition to defect formation, contributes to atom migration.

Besides, dislocation amount in Fe layers increases with the deformation time. It contributes to the appearance of grain structure, and this structure begins more dispersive with increasing of deformation time (Fig. 6).

By the way, dislocation formation in Fe is much higher in a case of thicker Fe layers. In this case two kinds of dislocations with Burgers vectors $b^1 = (a/2)\langle 111\rangle$ and $b^2 = a\langle 100\rangle$ appear in Fe layers. Those dislocations in Fe in addition to dislocations in Al, formed through the deformation process, can promote the accelerated mass-transfer on the phase interface Al–Fe forming the diffusion zone and contributing good adhesion of alloyed layer with the base material. Besides, the redundancy of vacancy formation, which occurs on the phase interface, contributes to the accelerating of diffusion processes in real crystals, but vacancy mechanism of diffusion is not high speeded as a dislocation mechanism and is not realized in the modelled samples due to short time of modelling.

4. CONCLUSIONS

The UIT processing of Д16 alloy by the Armco-iron pin leads to the formation of alloyed layer on the surface of base material. The thickness of alloyed layer increases with the treatment duration and is 12.7 μm after 90 s of treatment and 18.1–18.5 μm after 180 s of treatment.

Impact treatment contributes to the formation of diffusion zone on the phase interface between aluminium alloy and Fe-alloyed layer, which provides better adhesion of alloyed layer with the base material. The thickness of the diffusion zone is mostly 3.1 μm after 90 s of UIT and 4.6 μm after 180 s of UIT.

The molecular dynamics research of atoms behaviour on the phase interface between f.c.c. structured Al and b.c.c. structured Fe under impact deformation showed that the phase interface is a source for the dislocation formation in both materials, which leads to the mutual atoms migration through the face interface and can contribute to the accelerated mass-transfer under impact treatment in the processed sample in addition to the redundancy of vacancy formation on the phase interface in real crystals.

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