Superlattices and Microstructures 46 (2009) 114–120

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Local electron structure and magnetization in β-$Fe_{86}Mn_{13}C$

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A R T I C L E I N F O

Article history:
Available online 20 January 2009

Keywords:
Frank–Kasper structure
Local electron structure
Spin-polarized electronic conditions

A B S T R A C T

The aim of the work is to elucidate the origin of magnetization presence in austenitic $Fe_{86}Mn_{13}C$ steel after dynamic loading.

The observation of microstructures in the region of transition from FCC austenitic $Fe_{86}Mn_{13}C$ steel to FK12 + FK14 type of Frank–Kasper tetrahedral close packed structure is described. We used the methods of optical microscopy, electron microscopy, electron diffraction and X-ray-diffraction to investigate the phase transition region. Changes of local magnetization were estimated by induction method.

To explain the magnetization origin of the sample consisting of austenite grains and intergranular layers, which have Frank–Kasper's structure (FK12 + FK14) typical of β–Fe–Mn, the local electronic structure has been investigated for intergranular layers. The local electron structure of FK12 and FK14 clusters have been simulated by method of self-consistent field to understand the nature of non-zero magnetization of the $Fe_{87}Mn_{13}$ alloy exposed by shock deformation. It was shown, that numbers of states with upward and downward spins are not equal. Therefore the occurrence of magnetization is possible.

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0749-6036/$ – see front matter © 2009 Published by Elsevier Ltd
doi:10.1016/j.spmi.2008.11.023

1. Importance of research

The importance of $Fe_{86}Mn_{13}C$ alloys (Hadfield's manganese steel) researches is determined by their wide use in machine industry as constructive materials. In this work we attempt to find out the physical nature of high shock viscosity of $Fe_{86}Mn_{13}C$ alloy, its mechanical and magnetic properties. The results of electron structure calculation may be used for the prediction and interpretation of local changes in the structure and of properties in materials with developed intergranular boundaries.

The aim of this work is to elucidate the origin of magnetization presence in austenitic $Fe_{86}Mn_{13}C$ steel after dynamic loading.

Problems:

1. Investigate intergranular, (interboundary) layers in thin films and volumetric specimens of $Fe_{86}Mn_{13}C$ alloy with invar effect;
2. Investigate the influence of dynamic loading on magnetic characteristics of both massive and film specimens of alloy;
3. Make the analysis of structural and magnetic transitions in alloy with invar effect;
4. Construct the local electron structure of $Fe_{87}Mn_{13}$ alloy using scattering wave method with the purpose to give qualitative explanation of steel magnetic properties at mechanical loading.

In this report the observation of microstructures in the region of transition from FCC austenitic $Fe_{86}Mn_{13}C$ steel to FK12+FK14 type of Frank–Kasper tetrahedral close packed structure [1] is described. We used the methods of optical microscopy, electron microscopy, electron diffraction and X-ray-diffraction to investigate the phase transition region. The tetrahedral close packed structure of FK12+FK14 type arose in intergranular space (at grain boundaries) from initial austenitic steel as a result of prolonged shock deformation.

The shock deformation of nanocrystalline material excites the temperature gradient and the movement of nanoparticles groups relatively to each other. As a result, re-organization of individual nanoparticles takes place. The phase transition resulted in the formation of pseudomonocrystals, both periodic and quasiperiodic. It can be observed in intergranular space.

The Frank–Kasper structure is forming at fast cooling in water from 1150 °C down to room temperature, and possesses high viscosity and plasticity at enough good durability typical for austenitic steels.

The most important features of alloy $Fe_{86}Mn_{13}C$ is high resistance to dynamic loadings (impact elasticity makes more, than 300 MPa s), and also its invar effect. The invar effect is an independence of the linear factor of expansion of temperature in the field of temperatures from −100 to +250 °C. The deformation as a result of shock loading can change the module of elasticity and magnetic structure of an alloy. Changes of local magnetization were estimated by Kerr's method.

The Illustration of $Fe_{86}Mn_{13}C$ bulk sample after dynamic loading of 3000 kg on testing hardness by Brinell's method is shown on Fig. 1. In the printed area from initial austenitic phase with the FCC-lattice, mechanochemical reaction with formation of Frank–Kasper's structures has taken place [2]. The film samples were evaporated on glass and NaCl substrates. Due to difference of temperature coefficient of expansion of form and substrate the strain about 5–10 GPa can appear. The picture of electron diffraction, received on transmission electron microscope from a film sample of $Fe_{86}Mn_{13}C$ is shown on Fig. 2. We can see a two-dimensional projection from three-dimensional quasicrystal structure with symmetry of the eighth fold. This picture is similar to the Amman–Binker lattice, which also has an eight-fold symmetry axis. In early work [3] analyzing the selected areas of diffraction picture from patterns. The authors show the transition from crystal sample to quasicrystal one in tetrahedral close-packed structure of Frank–Kasper. We found the presence of the Frank–Kasper's tetrahedral close-packed structure FK12+FK14 types in nanocrystalline films of $Fe_{86}Mn_{13}C$.

Magnitude of coercive force was measured by induction method on bulk specimens. Hysteresis loop found far from loaded area is illustrated on Fig. 3, in loaded area — on Fig. 4. It can be seen that magnetization is heterogeneous on a sample.

From the work of H. Sidhom and R. Portier [4] it is known, that intergranular interface layers with icosaedral structures can exist in the stainless steel with austenitic structure. The icosahedral structure is one of four Frank–Kasper's structures, i.e. close packed tetrahedrons FK12 type.

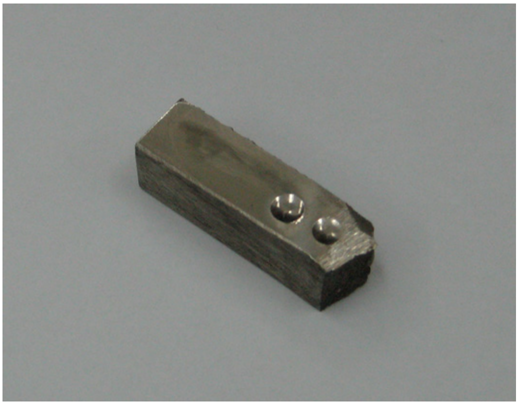

Fig. 1. The Illustration of $Fe_{86}Mn_{13}C$ sample after dynamic loading 3000 kg on installation of test of hardness by Brinell's method.

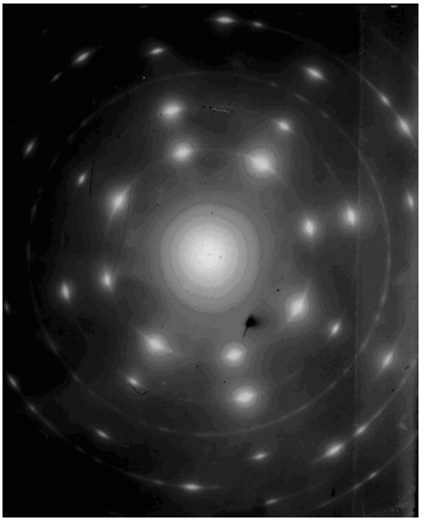

Fig. 2. The picture of electron diffraction, received from thin film sample of Fe–Mn–C, of two-dimensional quasicrystal which also have an eight-fold symmetry axis.

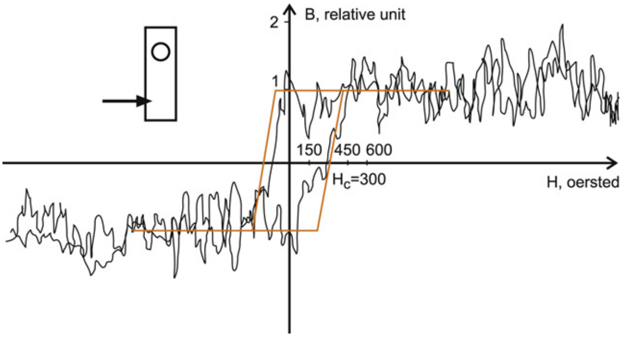

Fig. 3. Measurement of coercive force far from marked area for bulk sample (Fig. 1).

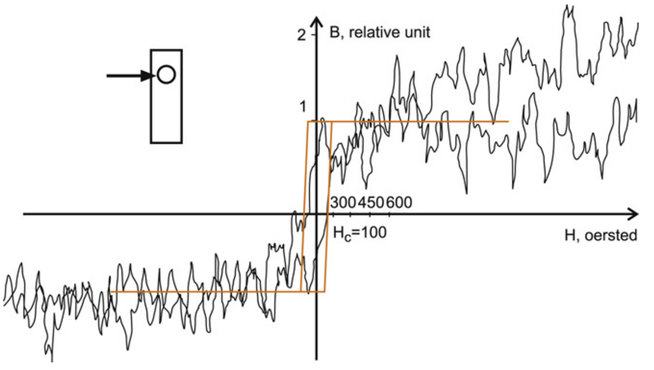

Fig. 4. Measurement of coercive force in marked area for bulk sample (Fig. 1).

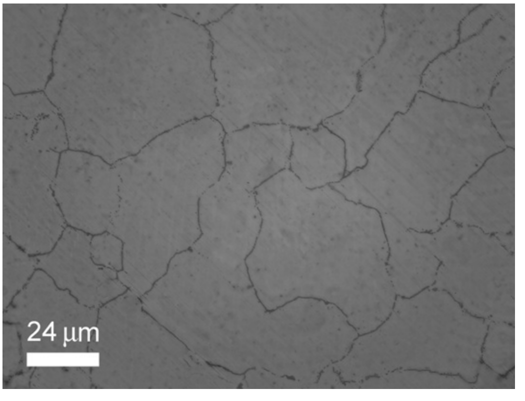

Fig. 5. Austenitic structure, usual for $Fe_{86}Mn_{13}C$ in an initial condition before loading.

An austenite structure is usual for $Fe_{86}Mn_{13}C$-steel in an initial condition i.e. before shock loading. We can see this structure on polished face specimens in optical microscopy. It is shown on Fig. 5. Structure of samples after long shock loading in an operating mode of rock-crushing machine can be seen on Fig. 6. Using the X-ray diffraction analysis, it can be seen, that the X-ray diffraction pictures received from a surface of steel $Fe_{86}Mn_{13}C$ sample, from an austenite grain (Fig. 7), — match the FCC structure. The wide dark layers between light grains of austenite have appeared. Diffraction of X-rays in the printed area turned out similar to X-rays diffraction picture received from intergranular layers of the steel subjected to long dynamic stressing. That corresponds to Frank–Kasper's structure. Diffraction pictures of $Fe_{86}Mn_{13}C$ sample received from intergranular layers, at the scanning of sample surface by X-ray beam is represented on Fig. 8 [5,6].

To explain the magnetization origin of the sample consisting of austenite grains and intergranular layers, which have Frank–Kasper's structure (FK12+FK14) typical of β-Fe–Mn, the local electronic structure has been investigated for intergranular layers. The local electron structure of FK12 and FK14 clusters have been simulated by method of self-consistent field [7,8] to understand the nature of non-zero magnetization of the $Fe_{87}Mn_{13}$ alloy exposed by shock deformation. For this purpose two cluster elements of a β-$Fe_{87}Mn_{13}$ cell have been chosen. These cells differ from each other by structure and number of atoms: 13 (FK12) and 15 (FK14) according to Frank–Kasper β-Fe–Mn type structure. The densities of spin-polarized electronic conditions of chosen nanoclusters, received by self-consistent field method are shown on Figs. 9 and 10. (Fermi-level is marked with dotted line.) On top half plane the density with downward spins is shown, in bottom half plane — upward spins. It can be seen that numbers of conditions with upward and downward spins are not equal. Therefore the occurrence of magnetization is possible.

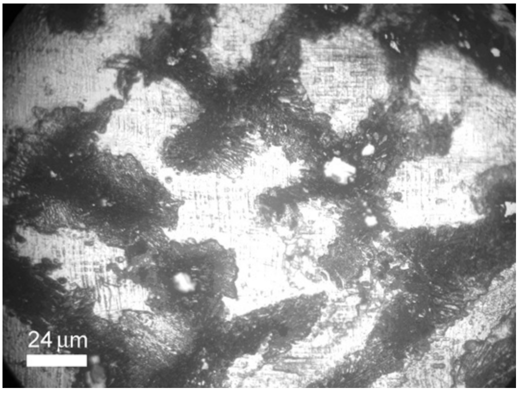

Fig. 6. Structure of samples after long shock stressing in an operating mode of rock-crushing machine (the wide dark layers have appeared between light grains of austenite).

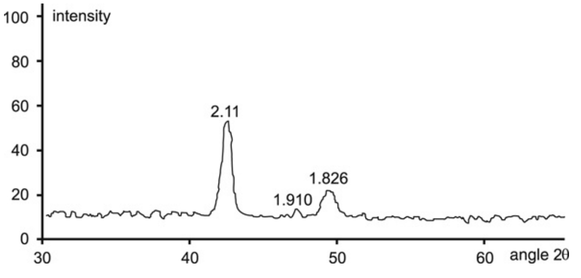

Fig. 7. Diffraction picture of X-ray received from a surface of $Fe_{86}Mn_{13}C$ sample, from an austenitic grain.

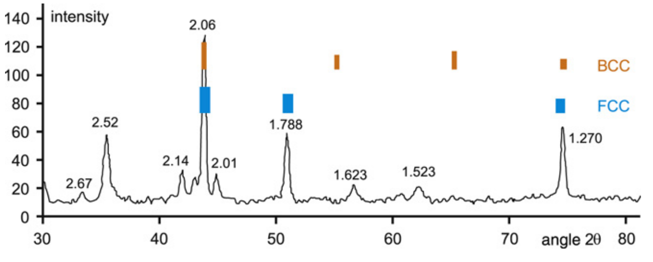

Fig. 8. Diffractogram of $Fe_{86}Mn_{13}C$ received from intergranular layers, at scanning a sample's surface by X-ray beam.

Differences in clusters structure and, as consequence, in potentials of their atoms and wave functions result in the different magnetic moment in local areas of the β-phase. We found out that the difference in the FK12 and FK14 cluster structure results in the different magnetic moment clusters. The spin-polarized calculation shows the value of magnetic moment $\langle\mu\rangle = 1.4\mu_B$/at in case of FK12 cluster and $\langle\mu\rangle = 0.5\mu_B$/at for FK14 cluster.

It is known that strains can trigger chemical reactions. This fact is very important: mechanochemistry is based on strain-induced chemical reactions (see Gilman [9]). The observed phase transition is accompanied by the appearance of non-zero magnetization, whereas austenitic $Fe_{86}Mn_{13}C$ steel is compensated antiferromagnetic. The $\acute{\alpha}$-phase of martensite was not found in this structure.

In our opinion, there are sufficient reasons to consider that the features of phase transition processes in localized regions of metal alloy with a self-assembling structure can be described in the framework of the modern shear transformation zone theory based on the excited-atom model

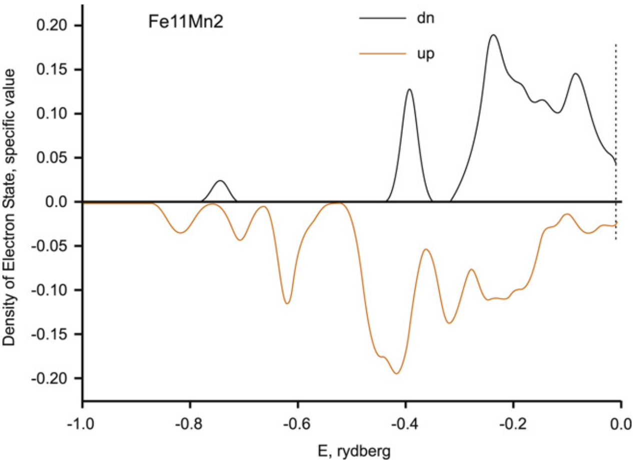

Fig. 9. Density of spin-polarized electronic conditions of a chosen nanocluster FK12, received by self-consistent field method.

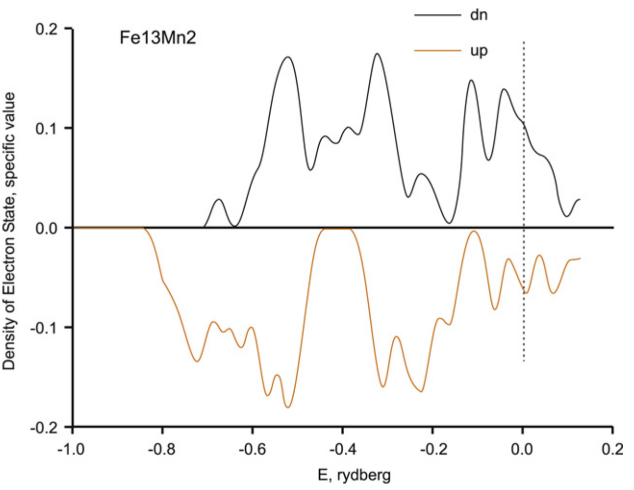

Fig. 10. Density of spin-polarized electronic conditions of a chosen nanocluster FK14, received by self-consistent field method.

[10,11]. This theory asserts that macroscopic deformation in non-equilibrium material is a result of local rearrangements due to the cooperative motion of molecules in mesoscopic domains. Plastic flow appears due to the creation and annihilation of the transformation zone which velocity linearly depends on strain. A dynamic model of super-Arrhenius relaxation in glassy materials was recently developed in [11]. It is based on a well-known liquid-like model [10]. Frank–Kasper's structure can be formed as a result of shear transformation zone movement in interborder layers [11]. As a result of tetrahedrally close-packed structures formation quasicrystal phases can appear.

2. Conclusions

1. In Fe–Mn–C alloy with invar consistent (Hadfield manganese steel) of bulk and film states the interboundary layers were found, which have Frank–Kasper structure FK12+FK14 of β-Fe–Mn type.
2. Magnetic characteristics of both bulk and film states of alloys are spontaneously changing under the action of dynamic stressing.

3. The local electron structure constructed by scattering waves method, qualitatively explains the magnetic properties during mechanical stressing.

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