

Iron Aluminides and Petr Kratochvíl

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Professor Petr Kratochvíl initiated a modern investigation of this class of materials in our country. He has been interested in various methods how to improve iron aluminides by alloying, precipitation and insertion of hard particles. He also restored the results obtained already in fifties of the last century in the development of so called PyroFerAl that was produced in Czechoslovakia and used, for example, for heat treatment installations. Professor Petr Kratochvíl has been cooperating with leading institutions for material research, for instance, with the Institute of Physics of Materials AS CR in Brno on creep studies or with the Technical University in Ostrava on material formation processes. Since aluminium is near the [nonmetals](#) on the periodic table, it can bond with metals differently than do other metals and hence the properties of iron aluminides, in particular, are different from the other intermetallics. These alloys can be also used as functional materials due to their magnetic properties. Iron aluminides are being developed for use as structural materials and/or cladding alloys in fossil energy systems. They have good high temperature mechanical properties and excellent corrosion resistance. These alloys offer relatively low material cost, conservation of strategic elements and a lower density than stainless steels, and thus they have a great potential for substituting steels at elevated temperatures. However, a wider use of these materials is partly hampered by their moderate ductility at ambient temperatures.

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1. Introduction

In this year we celebrate a round anniversary of a long-lasting member of the Department of Physics of Materials, Faculty of Mathematics and Physics, Charles University in Prague, Prof. Petr Kratochvíl. As a young scientist he was working at the Cavendish Laboratory, University of Cambridge, United Kingdom of Great Britain and at Institut für Materialphysik, Georg-August-Universität, Göttingen, Germany. In our country he collaborates intensively with several research institutions on the mechanical properties and structure of materials. In 1961 he contributed by a chapter on nucleation of dislocations during crystal growth to the first Czech book on dislocations in solids [1] where the theory of dislocations was summarized by Dr. František Kroupa and the experimental study of dislocations by Dr. Bohdan Šesták. Together with Prof. Pavel Lukáč and Doc. Boris Sprušil he published in 1984 the textbook *Introduction to Physics of Metals* [2] widely used by students of solid state physics.

Leading topic of his research is surely iron aluminides. Professor Kratochvíl restored the knowledge of the Czech alloy PyroFerAl [3], heat resistant material with applications, e.g., for various parts of furnaces, that can replace

more expensive materials highly alloyed with chromium and nickel. Besides his own research, he has also been active in dissemination of scientific result. From the establishment of the journal *Intermetallics* in 1993, he was for several years a member of its Editorial Board [4].

2. High-temperature study of iron aluminides

Professor Kratochvíl started to investigate then already popular iron aluminides [5] around 1992 by pointing the importance of two-phase region avoided by composition Fe–28 at.% Al and chromium addition. The first experiments were focused on sample composition [6] and lattice defects [7], the mechanical properties were later linked with the phase composition and ordering [8]. For instance, it was shown that the anomalous temperature dependence of the yield stress is related to the growth of DO_3 ordered domains into the $B2$ ordered structure [9]. The technical processes of the sample preparation and cerium addition were the next steps in his research [10]. High-temperature properties of Fe–Al system with alloying elements and particles added to improve this alloy behaviour were studied in cooperation with the Institute of Physics of Materials, AS CR Brno, Drs. Ferdinand Dobeš and Karel Milička, the Laboratory of Material Properties at High Temperatures, SVÚM Běchovice, Drs. Jan Hakl and Tomáš Vlasák, and the Department of Material Science, Technical University Liberec, Drs. Pavel Hanus and Věra Vodičková. So called “coarse grained superplasticity” was observed [11] and was explained by lattice dislocation movement along the elongated grains

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that yields the main contribution to the total strain. The effect of various additions as carbon and silicon was also investigated. Both carbon and silicon improve the creep resistance but the effect of silicon was more significant [12]. A special attention was paid to zirconium additions [13–16]. It was shown that the material with such additions can easily be rolled to prepare sheets for high temperature corrosion protection.

3. Technological applications of iron aluminides

Conditions for optimization of the hot rolling process of the iron aluminide Fe–28.4Al–4.1Cr–0.02Ce (at%) were investigated in [17]. Parameters that must be controlled for rolling are temperature, strain, and strain rate. All these quantities influence the deformation behaviour, which was described using a model of deformation resistance and the observed structure originated during hot rolling.

Casting in ultrasound field was tested to improve the microstructure of aluminides. An ultrasonic device was designed in cooperation with the Technical Universities in Liberec and in Ostrava [18]. The efficiency of ultrasonic vacuum casting, based on the influence of the acoustic cavitation on the solidification of the melt, was manifested by a refined microstructure of the prepared iron aluminides Fe–40 at.% Al with addition of C or Zr and B.

4. Magnetism in iron aluminides

Anomalous dependence of the lattice constant of iron-rich iron–aluminium alloys [19] has been found not to result from the order–disorder structural transformation but from the change in magnetism [20]. The anomalous volume dependence on composition can be removed when the magnetism is switched off in the frame of *ab initio* model based on the density functional theory.

A large number of authors from several institutions in different countries (the Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, and IFW Dresden (Germany), the Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut (Switzerland), the Department of Materials Science and Engineering, Royal Institute of Technology (Sweden), the Research Center, Philip Morris (USA), the Institució Catalana de Recerca i Estudis Avançats (ICREA), Institut Català de Nanotecnologia, and Departament de Física, Universitat Autònoma de Barcelona (Spain)) have proposed a new method for magnetic data storage and other applications in electronics [21]. Atomically ordered Fe–40 at.% Al alloy (*B2* structure) is paramagnetic at room temperature, however, when locally disordered by means of focused ion beam it becomes ferromagnetic. The disordered domains (ferromagnetic dots) can be fully removed by annealing.

5. Dislocation in iron aluminides

The shortest lattice vector in the ordered *B2* structure is $\langle 001 \rangle$, however, it is not always the Burgers vector of full lattice dislocations that carry the plastic deformation. The exceptions are the CuZn and FeAl systems where the $\langle 111 \rangle$ slip occurs. The first of them is known for its large elastic anisotropy (CuZn 10.42) but the latter one has the elastic anisotropy comparable with the other systems as CoTi or NiTi (FeAl 2.36, CoTi 2.42, NiTi 2.73) where the $\langle 001 \rangle$ slip is observed. The transition-*B2*-melt temperatures that indicate the magnitudes of the ordering and antiphase boundary energies are also very close to each other (FeAl 1310 °C, CoTi 1325 °C, NiTi 1310 °C), contrary to CuZn where the transition *B2*-bcc is observed at relatively low temperature of 460 °C, not occurring at the other three systems. Nevertheless, the dislocation core structure controlling dislocation behaviour is determined by a complex interplay of several factors: the Burgers vectors of partial dislocation, the energies of stacking-fault-like defects and the elastic constants, all of them determine the dissociations widths. Hence, the FeAl system is unusual due to a special combination of its parameters different from CuZn [22, 23]. For more information on dislocation behaviour in different types of intermetallics see [24, 25].

6. Conclusions

This report does not cover all the important results of Prof. Petr Kratochvíl activity, it is only a short notice to commemorate his achievements. The iron aluminides are regularly discussed at the meetings organized by Max-Planck-Institut für Eisenforschung, Germany, and at other international conferences on intermetallics, for example [26, 27].

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