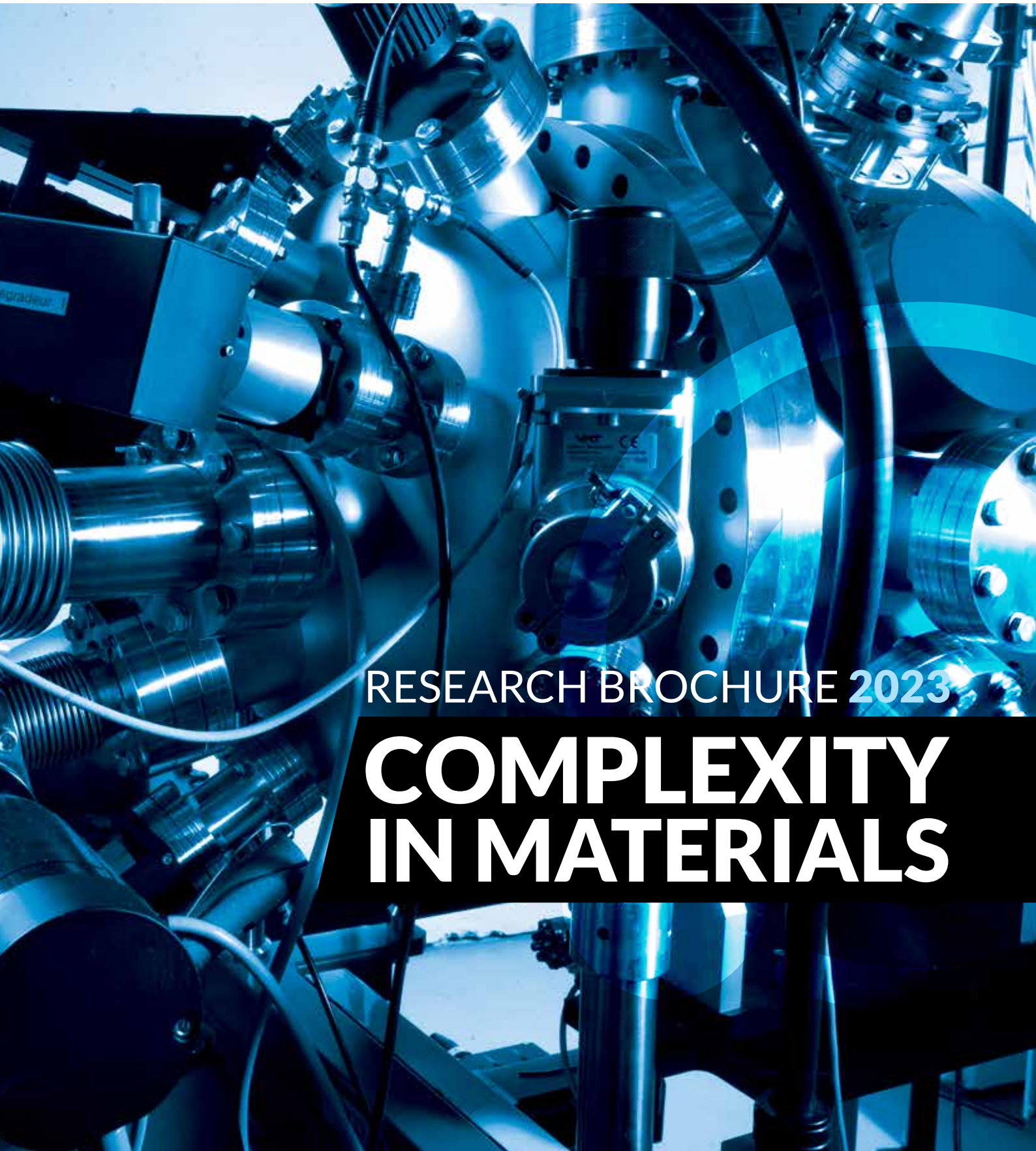
NOMATEN

Centre of Excellence in Multifunctional Materials
for Industrial and Medical Applications



RESEARCH BROCHURE 2023

COMPLEXITY IN MATERIALS

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GENERAL SUMMARY BY PROF. MIKKO ALAVA

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RESEARCH GROUP LEADER: COMPLEXITY IN MATERIALS

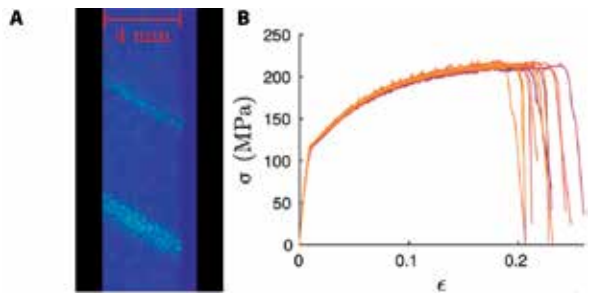
The modeling of materials for harsh environments presents many challenges: the end-properties such as strength or resistance to irradiation and high temperatures depend on material composition and on the processing, a well-known fact for metal alloys and also for amorphous, glassy materials. The work in this Research Group has concentrated on two main focus questions, the mechanical properties on one hand and on the application of machine learning and data science to data sets, both experimental and simulation-based ones. This second application area opens up a wide variety of interesting collaboration possibilities with the other Center of Excellence groups and with external collaborators.
The physics of plasticity in complex alloys exhibits fascinating features, including the Portevin-Le Chatelier effect and its cousins. In PLC, the response of a sample or specimen to loading becomes jerky, which results from the localization of plastic deformation in “bands” or waves. This is of course a detrimental effect – PLC is met in many different metal alloys from steels to aluminum -based ones, and clearly for instance if used in aircraft structures there is the risk of catastrophic failure. The origins of this behavior are since long known to originate in the alloy composition. The key ingredient is the presence of so-called solute atoms, which move around in the crystal structure and interact with the carriers of plastic deformation, dislocations. This movement depends on temperature, and thus to create such instabilities the combination of temperature and the rate of loading (“strain-rate”) must be met – or avoided.

SCIENTIFIC DEVELOPMENTS

In our work "Propagating bands of plastic deformation in a metal alloy as critical avalanches" we took a novel angle on studying and explaining what happens in the PLC. The work is based on imagining that each of the deformation bursts is an "avalanche", a short intermittent event. We used for a rather typical aluminum alloy image analysis to follow the propagation of the PLC deformation bands. These look with sufficient accuracy and statistics like random walkers in a landscape, that is complicated by the disordered structure of the metal including the solutes.

We could show how a model can be built such that it accounts for the necessary metallurgical detail including the strain-hardening of the alloy. What these results mean is that each metal alloy exhibiting propagating PLC bands should be described by our model, but with different parameters in each case. This advance leaves us with a number of unanswered questions. For practical materials design the question becomes at which strain rate these violent bands appear, and below which the material behaves in a more friendly manner.

Features of deformation bands from speckle images
Figure A: *The raw subtracted speckle images showing two simultaneous PLC bands (top one during nucleation)*
Figure B: *The stress-strain curves showing the responses of the samples and the serrations*



An important materials science problem that couples functional properties, materials design or selection, and fundamental science is fracture. In many real world cases what we expect to see is the gradual growth of small flaws in a specimen, under varying loads and this is what defines fatigue fracture. The life-time of real-world structures or laboratory samples is governed by many features from the "fatigue protocol" or load history to environmental effects to the character and quality of the material. From the fatigue fracture mechanics viewpoint the important timescales are what it takes to nucleate "the" crack and how much time it takes to for the crack to grow to a catastrophic size. What we know in practice of this crack growth process is that it is very often described by the empirical relationship called the Paris-Erdogan -law, which summarizes in a simple relationship whether the growth is fast or slow.

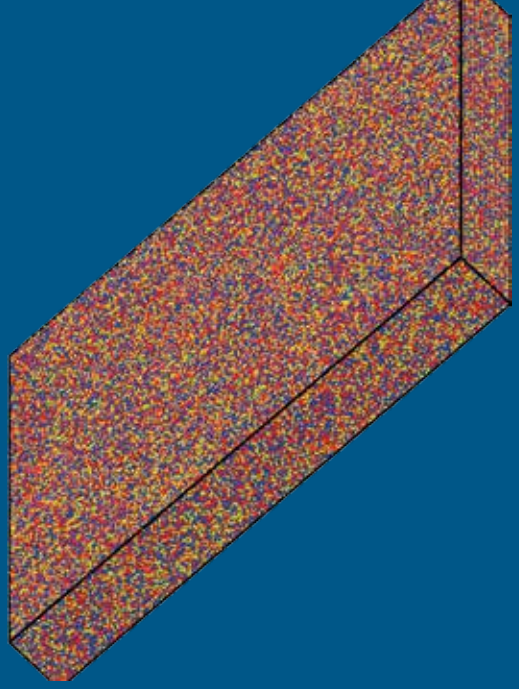
We studied in our paper "Fatigue crack growth in an aluminum alloy: Avalanches and coarse graining to growth laws" the fatigue process from the view point of basic fracture physics. Experiments measuring the Paris' law indicate that the growth rate or law is "an average" and is accompanied by variations and fluctuations around the average growth. This turns out to mean – after careful experiments – that the fatigue crack tip undergoes stop-and-go motion or in other words sometimes the crack growth is stalled, to be then followed by spurts of faster growth. The main discovery to explain the Paris' -like growth from our work is that the average growth and thus the sample/material lifetime are dictated by the small scale plasticity, which sets the maximum rate by which the crack grows. There are exciting directions of understanding the fatigue further by combining our analysis with crack sub-surface studies of the plasticity by Scanning Electron Microscopy or by looking at the texture of the crack surface. These methods would allow to look at the cyclic plasticity and what kind of traces it leaves (under the surface, since plastic deformation extends to the metal bulk and by signatures of cavitation or void formation ahead of the crack tip).

So-called High-Entropy Alloys (HEAs) are now at the forefront of metallurgy and materials design. The main concept here is the famous Cantor alloy, in which five metallic elements are mixed into an equimolar alloy. HEAs are thought to have a great potential as the metallic materials of the future since roughly equal mixtures bring thermodynamic stability – the alloy does not develop internal phases or phase separate – and since their complex structure offers resilience. HEAs maintain often their physical and chemical properties up to very high (operating)

temperatures and are in particular a playground for looking better and better mechanical properties, stiffness and trength.
The two main problems that we face when doing research on these materials are how to process and make them, a traditional one, and how to find the best compositions? It is not unreasonable to think about changing the constituent species one by one or shifting the mixing ratios of the elements from a democratic mixture if this allows for better properties or might be of advantage in the material processing, but we get hit back by the astronomically large search space in which to look for better compositions.

The main modeling approach to the reason why HEAs are a promising solution for tougher metals is an “effective atom” description, where the dislocations in the alloys interact with the disordered atomistic neighborhood. This so-called pinning makes it so that the dislocations get stuck unless one applies large enough stresses so that they move and the material yields. The design of HEAs would be thus easy, but our idea was that this is not enough, one can do better. In the article “Edge dislocations in multicomponent solid solution alloys: Beyond traditional elastic depinning” we studied a number of HEA compositions by numerical modeling to check the validity of recent theory for a number of alloy candidates. The important physical detail in this work comes from the fact that the Face-Centered Cubic (FCC, iron-like) alloys have dislocations that split for the convenience of lowering their energy into two so-called partial dislocations. Our result is simply to state, the final yield stress or depinning stress of the FCC dislocations is actually much higher in some cases than expected: the alloys are stronger.
This is since the two partial dislocations are quite good in finding ways of getting pinned in unison, so larger stresses are required. The process by which this place is according to our modelling quite complex, so we plan to extend our work by summarizing it by detailed studies.

The range of alloys of modern interest also includes the so-called Medium Entropy Alloys: just mixing three elements may be sufficient to come up with interesting properties and for the sake of fundamental studies three or four element compositions are of course easier to comprehend than those with five or even more elements.



The classical toolbox for these MEAs consists of Iron, Chromium, Nickel and Cobalt due to their similarities as metals, but thhaen one may consider various substitutions to this set. The two main ideas that research follows in order to improve the alloy mechanical properties are both about the control of the material on the atomistic level.

The number one idea is to create internal stresses by the introduction of element(s) that have simply as big a size/elastic mismatch with the rest of the alloy species as possible. Thus we may ramp up the level of such stresses. The other possibility is to create alloys that are not completely random: so-called Short-Range Order. SRO gives a similar possibility of making the structure in which dislocations move more complex and frustrated, which might increase the resistance to dislocation movement and thus increase the yield stress.

In our work “Atomistic simulations of dislocation plasticity in concentrated VCoNi medium entropy alloys: Effects of lattice distortion and short range order” we tackle this design problem by looking at the case of controlling the material properties with Vanadium. It has been widely speculated to be an advantageous composition ingredient due to the fact that the atoms are “big” compared to the other composition partners. This we then confirm by looking at various mixtures and changing the detailed mixing ratios with Cobalt and Nickel.
We then also look at the possibility of improving yield strength further by creating “in silico” – in the simulations by a refined technique – samples with SRO. All in all, our work shows the potential of materials design by careful simulation work.

SELECTED PAPERS ABSTRACTS

Fatigue crack growth in an aluminum alloy: Avalanches and coarse graining to growth laws

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19 November 2021;
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In fatigue fracture the crack growth is slow and in many materials exhibits apparent self-similarity as expressed by the dependence of the growth velocity on a stress intensity factor that grows with the crack size. We study the intermittency of fatigue crack dynamics in aluminium alloys by optical tracking. A power-law distribution of crack tip jumps is found with an exponent close to two and a cutoff which increases with time or crack propagation. The cutoff is related to the crack velocity. We show how such a distribution evolves or coarse grains with the scale of observation or time window. The correlations of the crack propagation imply short-range memory effects in the underlying dynamics. Our results show universal features of fatigue cracks and how these lead to the crack growth and failure in material samples.

Propagating bands of plastic deformation in a metal alloy as critical avalanches

SCIENCE ADVANCES 7 Oct 2020; Vol 6, Issue 41;
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The plastic deformation of metal alloys localizes in the Portevin–Le Chatelier effect in bands of different types, including propagating, or type "A" bands, usually characterized by their width and a typical propagation velocity. This plastic instability arises from collective dynamics of dislocations interacting with mobile solute atoms, but the resulting sensitivity to the strain rate lacks fundamental understanding. Here, we show, by using high-resolution imaging in tensile deformation experiments of an aluminum alloy, that the band velocities exhibit large fluctuations. Each band produces a velocity signal reminiscent of crackling noise bursts observed in numerous driven avalanching systems from propagating cracks in fracture to the Barkhausen effect in ferromagnets. The statistical features of these velocity bursts including their average shapes and size distributions obey predictions of a simple mean-field model of critical avalanche dynamics. Our results thus reveal a previously unknown paradigm of criticality in the localization of deformation.

Plastic yielding and deformation bursts in the presence of disorder from coherent precipitates

August 2020 Physical Review Materials 4(8); DOI:10.1103/PhysRevMaterials.4.083602

Alloying metals with other elements is often done to improve the material strength or hardness. A key microscopic mechanism is precipitation hardening, where precipitates impede dislocation motion, but the role of such obstacles in determining the nature of collective dislocation dynamics remains to be understood.

Here, three-dimensional discrete dislocation dynamics simulations of fcc single crystals are performed with fully coherent spherical precipitates from zero precipitate density up to pp=1021m−3 and at various dislocation-precipitate interaction strengths. When the dislocation-precipitate interactions do not play a major role, the yielding is qualitatively the same as for pure crystals, i.e., dominated by "dislocation jamming," resulting in glassy dislocation dynamics exhibiting critical features at any stress value.

We demonstrate that increasing the precipitate density and/or the dislocation-precipitate interaction strength creates a true yield or dislocation assembly depinning transition, with a critical yield stress. This is clearly visible in the statistics of dislocation avalanches observed when quasistatically ramping up the external stress, and it is also manifested in the response of the system to constant applied stresses. The scaling of the yielding with precipitates is discussed in terms of the Bacon-Kocks-Scattergood relation.

FUTURE PLANS

In the future the team will make a concentrated effort to drive new materials development at NOMATEN. We shall do this in collaboration with the other groups – the research shall be excellence-oriented, in that we solve key issues in modern materials science for challenging applications, but also done in a loop including models, experiment, and material informatics. This kind of holistic approach allows us to collaborate widely along the axis between fundamental research and solving specific industrial problems.

One of the most promising approaches is application of machine learning and data science to data sets, both experimental and simulation-based ones. Thanks to such developments we expect valuable collaborations with other NOMATEN's research groups and external partners.

The big picture is about the long-term potential as NOMATEN starts to produce experimental datasets for various advanced materials and the key concept is the combination of workflows for data analysis with Open Data.

Figure: CIŚ computer cluster at NCBJ, that helps Complexity in Materials research group perform its' research


COMPLEXITY
IN MATERIALS