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# MODELLING OF DEFORMATIONS ASSOCIATED WITH TYPE-II RESIDUAL STRESSES IN SINTERED Nd-Fe-B PERMANENT MAGNETS

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**Abstract**

*This study focuses on the modelling of the microstructure of Nd-Fe-B-based permanent magnets with inclusions of various shapes using the OOF2 software. Nd-Fe-B magnets are key components in renewable energy technologies, particularly in electric vehicles and wind turbines. However, their production poses technological challenges, notably due to the reliance on imported rare-earth elements.*

*The objective of this research is to analyse residual stresses and misfit strains in polycrystalline structures with different types of inclusions (specifically copper, Cu, in the form of spherical and triangular particles), which arise as a result of thermal processes and structural phase interactions.*

*Using the finite element method implemented in OOF2, numerical models were constructed to evaluate the influence of microstructural parameters on the magnetocrystalline anisotropy and coercivity of the magnets. The results obtained may be utilised to optimise manufacturing processes and enhance the performance of Nd-Fe-B permanent magnets.*

**Keywords:** Nd-Fe-B magnets, microstructure, residual stress, misfit strain, OOF2, magnetocrystalline anisotropy, coercivity, rare-earth elements, inclusions, modelling.

Rare-earth-based permanent magnets, particularly neodymium-iron-boron ($Nd_2Fe_{14}B$), are indispensable components in modern technologies aimed at the advancement of green energy. They are widely used in electric vehicle motors, wind turbine generators, and other high-tech devices that require high magnetic energy density and stability. Due to their unique magnetic characteristics, sintered Nd-Fe-B magnets exhibit high coercivity and remanence. However, their microstructure is complex, and their magnetic properties are highly sensitive to microstructural features.

It is well known that during powder sintering and subsequent annealing, secondary phases form in the intergranular regions and triple junctions. These phases consist of neodymium, copper, and compounds involving iron, oxygen, boron, and other elements [1]. Such inclusions generally exert a detrimental effect on the magnetic properties of the bulk material, both due to their intrinsic physical properties and due to mechanical interactions with the main phase. These mechanical effects manifest as residual stresses and type-II strains that arise at grain boundaries during thermal processing, due to mismatches in thermal expansion coefficients, phase transformations, and related factors.

Variations in atomic spacing within the crystal lattice associated with such stresses and strains can significantly alter the magnetocrystalline anisotropy of an otherwise stress-free crystal, directly influencing the magnetic properties of the material [2–7].

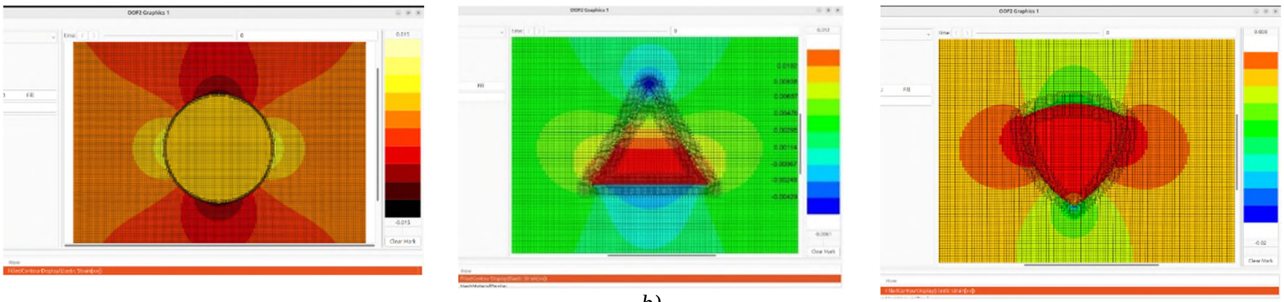
The accurate prediction of residual strains presents several challenges, primarily due to the complexity and uniqueness of the microstructure – such as grain size and shape, intergranular phase distribution, crystallographic orientation, and the morphology of inclusions. Additionally, it is difficult to precisely determine the physical and mechanical properties of the secondary phases, including volume change coefficients, thermal expansion, and elastic moduli.

A detailed analysis of selected microstructural scenarios characteristic of sintered Nd-Fe-B magnets, alongside systematic accumulation of data, will not only enable estimation of residual strains, but also contribute to the development of integrated models for structure optimisation, thermal treatment regimes, and magnet design.

It is evident that analytical methods possess significant limitations and can be applied only to simplified or idealised cases [4]. Approaching realistic scenarios necessitates the use of numerical techniques and specialised software tools.

In this study, the mechanical state of polycrystalline Nd-Fe-B magnets containing various types of inclusions was modelled using the OOF2 computational package. This software enables simulation of the stress–strain state in polycrystals based on real or synthetic microstructural images [8, 9]. Accordingly, the work investigates the influence of inclusion shape and orientation on the distribution of residual stresses and localised strains.

Artificial microstructures of Nd-Fe-B crystals were modelled with inclusions made of a secondary material, represented by shapes commonly found in actual sintered magnets – such as spheres and triangles of varying geometries (Figures 1, 2). The model geometry was constructed to reflect different inclusion morphologies, allowing a comparative analysis of residual stress distributions across the various scenarios.



*a)* *b)* *c)*

**Figure 1.** Strain distribution in the Nd-Fe-B magnet structure with copper (Cu) inclusion in the form of a spherical element (a), an equilateral triangular element (b), a curved convex triangular element (c)

The physical and mechanical properties of the primary Nd-Fe-B phase (stiffness matrix, coefficients of thermal expansion) were taken from literature [10]. The crystal orientation was set to (001), with the vertical axis aligned accordingly. The material properties of the inclusions were assumed to correspond to pure copper, as copper represents a plausible inclusion scenario with well-established material parameters.

Thermal strains resulting from cooling after sintering and annealing (from 500 °C) were considered in the simulations. These were accounted for using the respective coefficients of thermal expansion, crystallographic orientation, and stiffness constants for each constituent material.

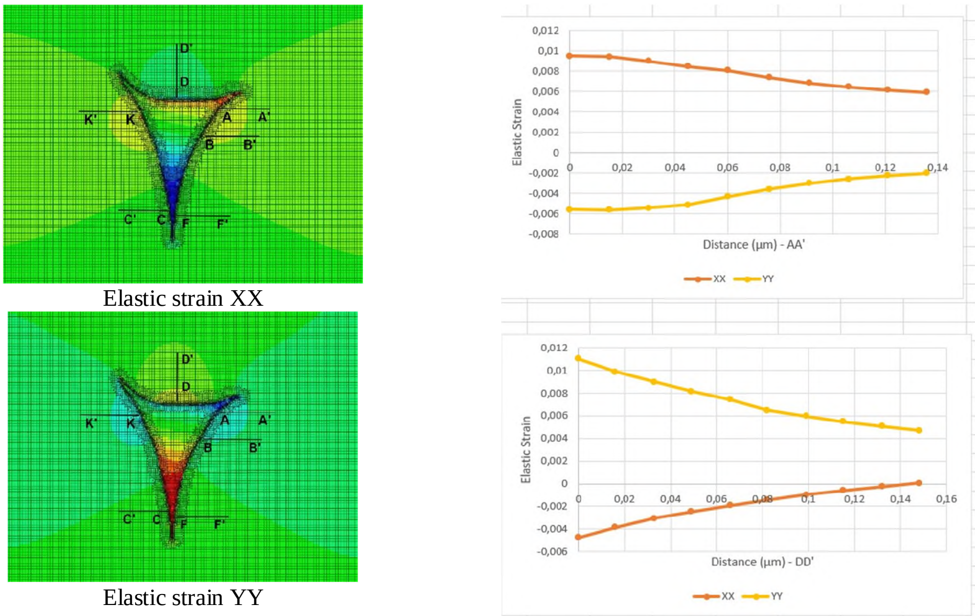



**Figure 2.** Strain distribution in the Nd-Fe-B magnet structure with copper (Cu) inclusion in the form of a curved concave triangular element. The shape of the inclusion elements was adapted from [2]

Analysis of the simulation results revealed that the geometry of inclusions significantly affects stress concentration. Triangular inclusions induce highly localised stress zones at their vertices, whereas spherical inclusions result in a more uniform distribution. This indicates that the inclusion shape may be a critical factor in designing microstructures with optimised magnetic performance.

## Conclusions

The conducted simulations demonstrated that accurate evaluation of the stress–strain state within the microstructure of Nd-Fe-B magnets reveals essential micromechanical factors influencing their magnetic behaviour.

Residual stresses arising from the mismatch in thermal expansion coefficients between Nd-Fe-B and copper lead to the development of localised deformations. The peak strain levels in the triple junction interface zones for the studied inclusion geometries ranged from approximately ±0.005 to ±0.015, depending on the inclusion shape and crystal orientation. This corresponds to an estimated impact on coercivity of around 10%, underlining the importance of mechanical effects in magnet design.

Considering the shape and spatial distribution of inclusions within the microstructure may serve as an effective engineering tool for optimising magnet performance while reducing dependence on rare-earth material content.

Future work will aim to extend the range of analysed inclusions by incorporating other material types and geometries, as well as to perform experimental validation of the numerical simulation results.

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# МОДЕЛЮВАННЯ ДЕФОРМАЦІЙ АСОЦІЙОВАНИХ ІЗ ЗАЛИШКОВИМИ НАПРУЖЕННЯМИ 2-ГО РОДУ В СПЕЧЕНИХ ПОСТІЙНИХ МАГНІТАХ Nd-Fe-B МЕТОДОМ СКІНЧЕННИХ ЕЛЕМЕНТІВ

**Анотація**

*У роботі розглядається моделювання мікроструктур постійних магнітів на основі Nd-Fe-B з включеннями різної форми за допомогою програмного забезпечення OOF2. Nd-Fe-B магніти є ключовими компонентами у технологіях відновлюваної енергетики, зокрема в електромобілях та вітрових турбінах. Однак їх виробництво супроводжується технологічними викликами, зокрема через залежність від імпорту рідкоземельних елементів.*

*Метою дослідження є аналіз залишкових напружень і місфітних деформацій у полікристалічних структурах з різними включеннями (зокрема міді Cu у вигляді сферичних та трикутних включень), що виникають унаслідок термічних процесів і структурної взаємодії фаз.*

*За допомогою методу кінцевих елементів, реалізованого в OOF2, було побудовано чисельні моделі, які дозволяють оцінити вплив мікроструктурних параметрів на магнітокристалічну анізотропію та коерцитивну силу магнітів. Отримані результати можуть бути використані для оптимізації виробничих процесів і підвищення ефективності постійних магнітів Nd-Fe-B.*

**Ключові слова**: Nd-Fe-B магніти, мікроструктура, залишкові напруження, місфітні деформації, OOF2, магнітокристалічна анізотропія, коерцитивна сила, рідкоземельні елементи, включення, моделювання.

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