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SuperFusion Group

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Modelling of radiation damage in superconductors for fusion applications



Politecnico
di Torino



EUROfusion

THE SUPERFUSION TEAM

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superfusion.org



Francesco Laviano
Associate Professor



Daniele Torsello
Tenure-track researcher



Federico Ledda
Defect modelling



Niccolò Di Eugenio
Machine Learning Potentials



Fabio Calzavara
Design optimization



Mattia De Stasio
Magnet modelling



Martina Casciello
Magnet modelling



Simone Severo
Experimental characterisation



Niccolò Gallino
Vortex dynamics



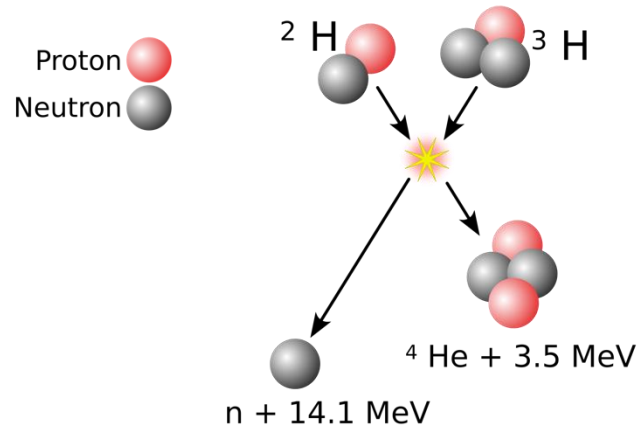
Francesco Mosciagiuri
Scientific Machine Learning



Pasquale Petrillo
Quench prevention

PHD STUDENTS

MOTIVATION: NUCLEAR FUSION



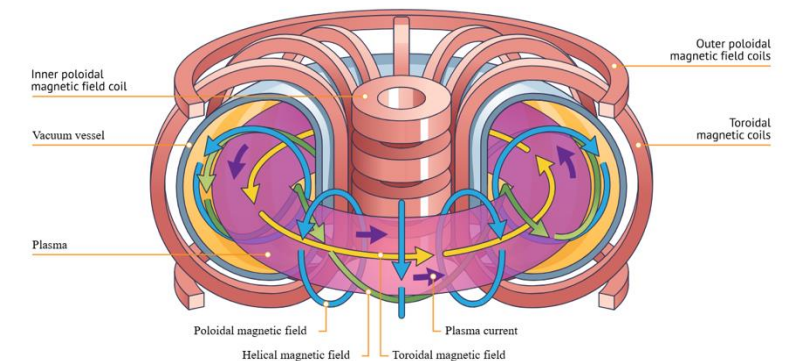
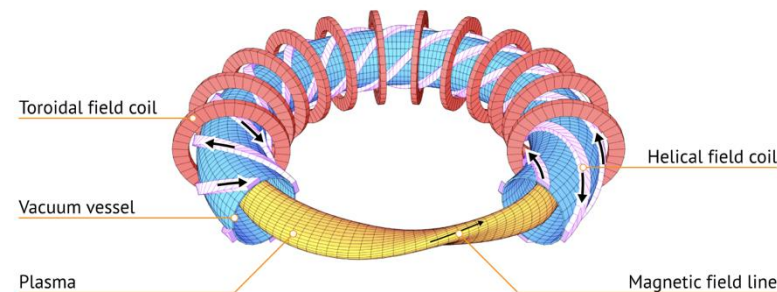
Nuclear reactions that, between light nuclei, release energy

Goal: Build reactors that harvest this energy

To obtain these reaction, nuclei and electrons must dissociate and create a **plasma**, which then needs to be confined → A **lot** of different proposals

MAGNETIC CONFINEMENT

Is the most researched and appears to be most promising for large-scale use



MOTIVATION



Kamerlingh Onnes,
1911

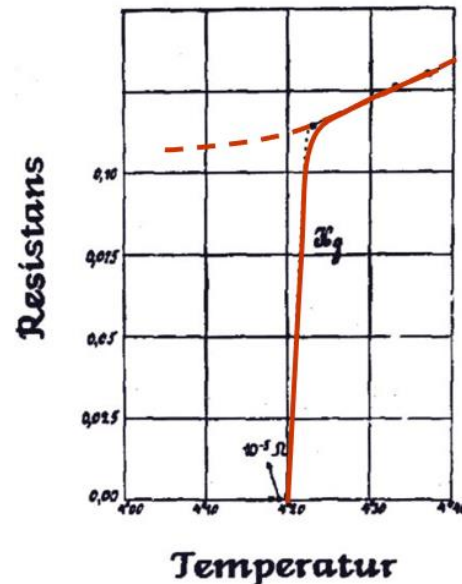
The magnetic fields need to be extremely strong (> 10 T) \rightarrow Need for very large **currents**



Perfect candidate materials: **superconductors**



Zero resistance



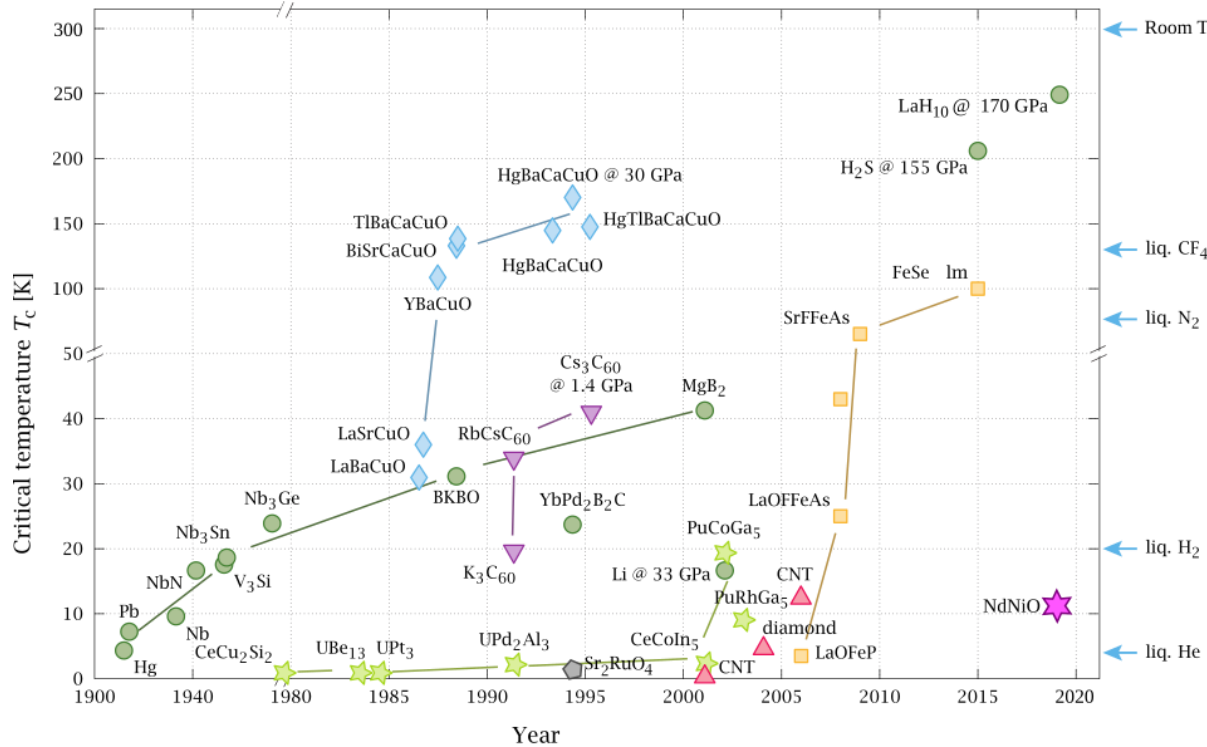
Properties:

- **Perfect conductivity:** zero resistance for electrical conduction
- **Perfect diamagnetism:** complete expulsion of an external magnetic field
- **Superconducting transition:** below certain critical parameters (temperature T_c , current density J_c , magnetic field H_c)

MOTIVATION

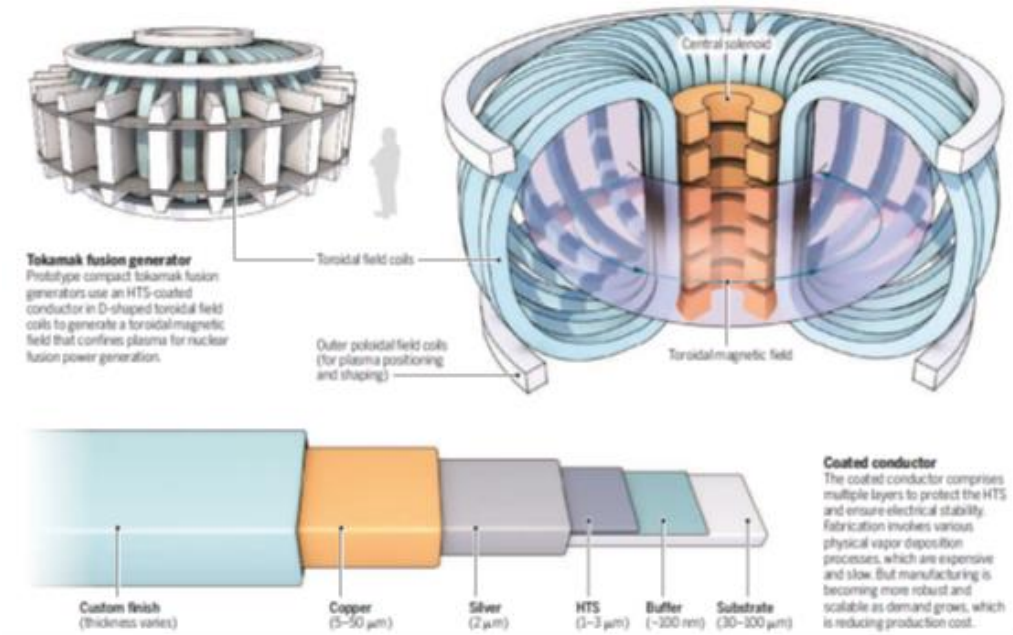
High Temperature Superconductors are able to sustain stronger fields and also have lower operational costs

Fabricated in **tapes** that are then wound to build the magnets



High-temperature superconductors in a tokamak fusion reactor

The development of nuclear fusion power generation, such as with compact tokamak fusion reactors, is driving the growth and commercialization of high-temperature superconductor (HTS)-coated conductors.



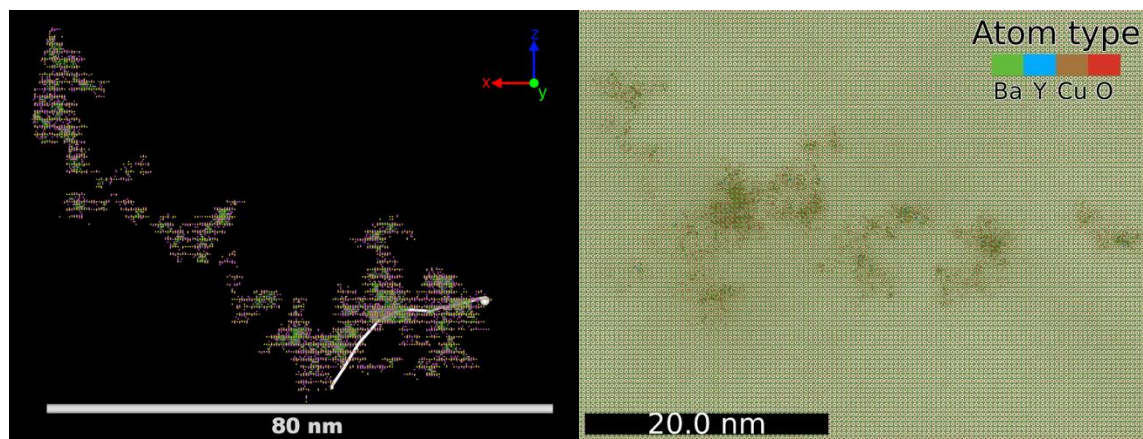
MOTIVATION

PROBLEM

Superconductivity is strongly relying on lattice crystal **structure**

Fusion-derived **neutrons** would irradiate magnets in reactors

Defects are introduced, that affect the superconducting performance



Torsello, et al. *SuST* (2022)

Linden, et al. *J. Microsc.* 2022

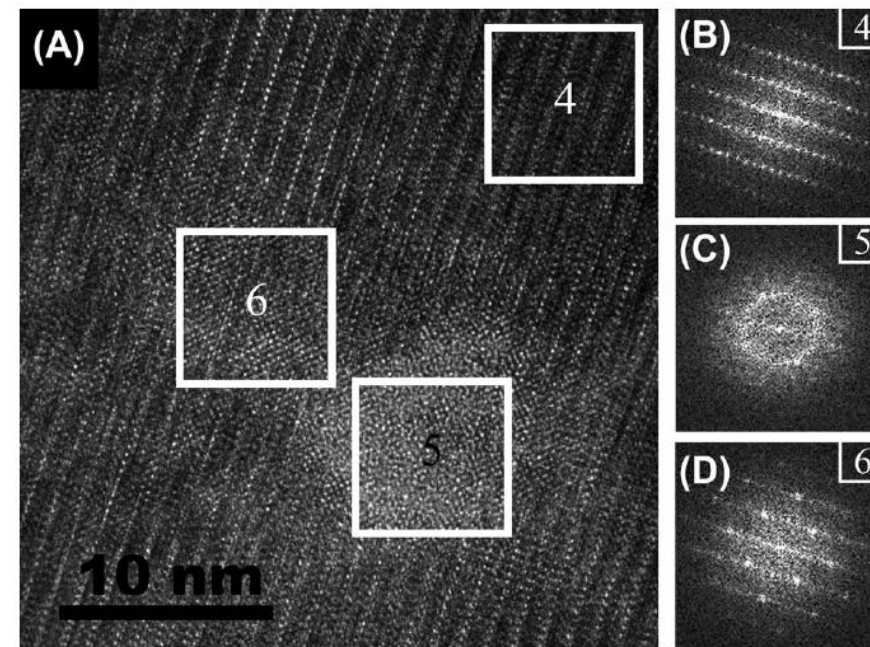
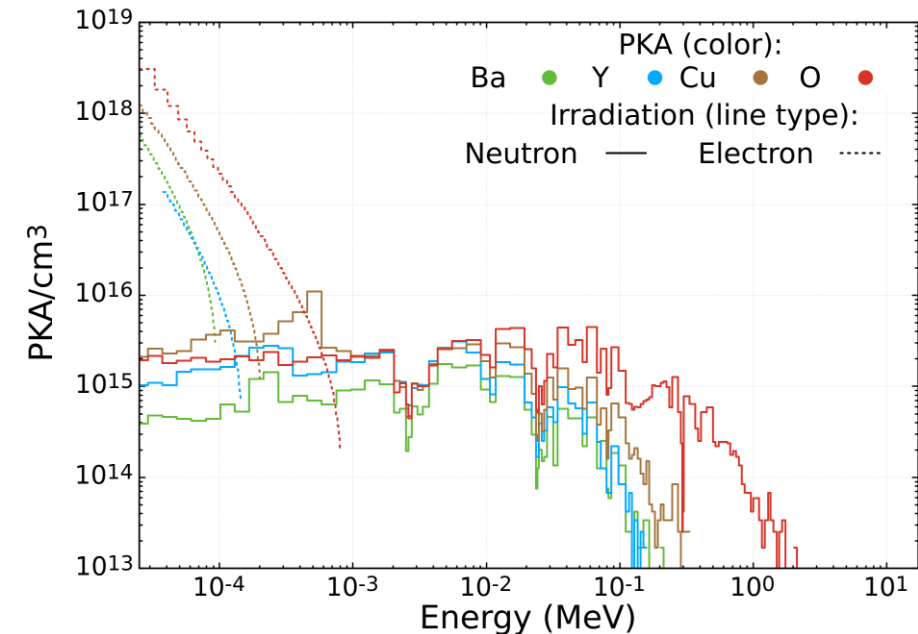
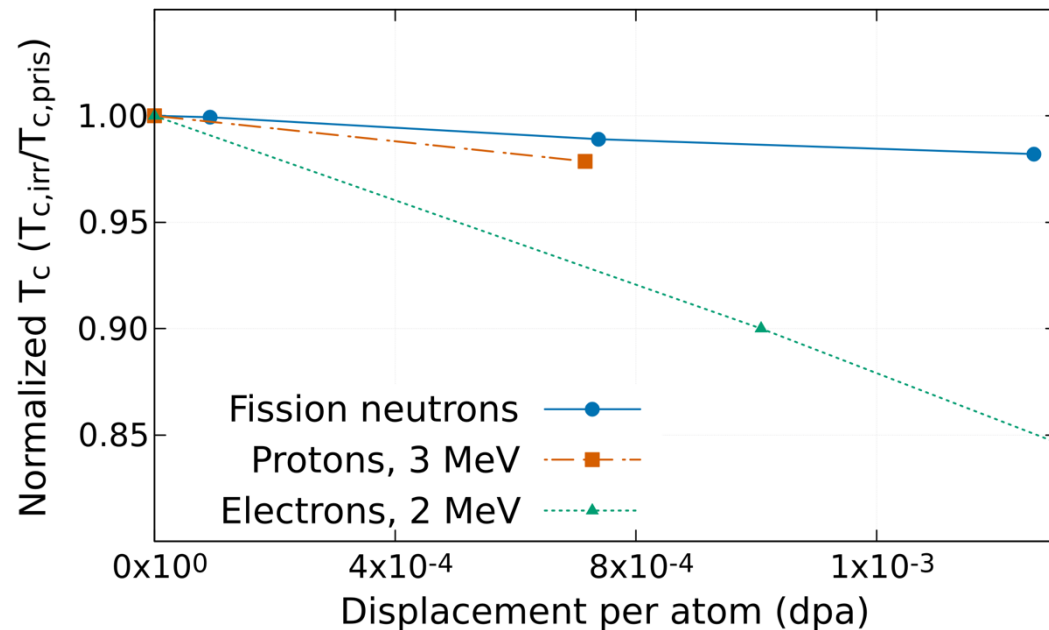


FIGURE 3 (A) HRTEM image taken along $[100]$ showing both an amorphous cascade core (5) and a distorted region (6) that can be distinguished from the undamaged crystalline matrix (4). (B)–(D) 7.48×7.48 nm window FFTs taken from regions 4, 5 and 6, respectively

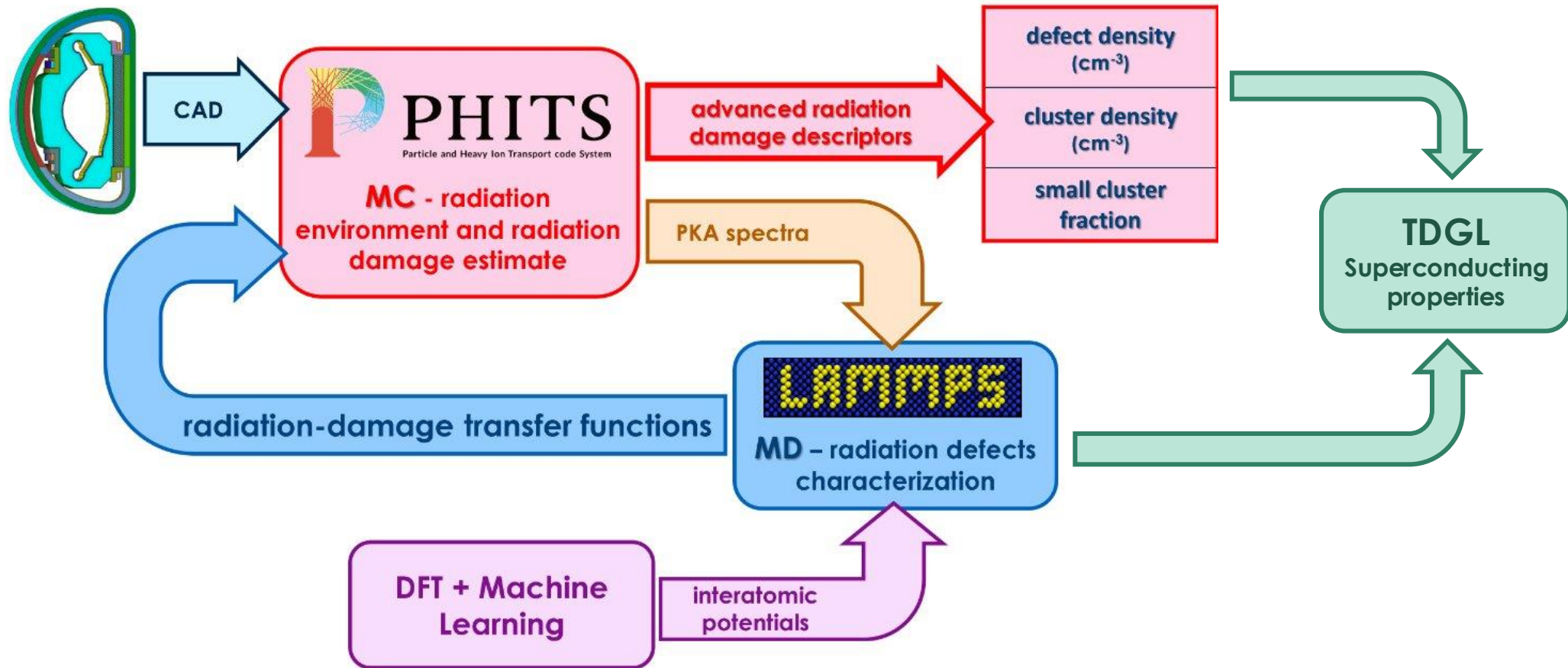
MOTIVATION

- Understanding the mechanism of superconducting properties degradation and **finding a reliable radiation damage threshold** are primary goals of ongoing research
- Current estimations based on straightforward Monte Carlo (**MC**) simulations, like **fluence or dpa, are not satisfactory** and might yield to misleading predictions
- Need for **universal descriptors of radiation damage** and **link to the superconducting properties**



WORKFLOW

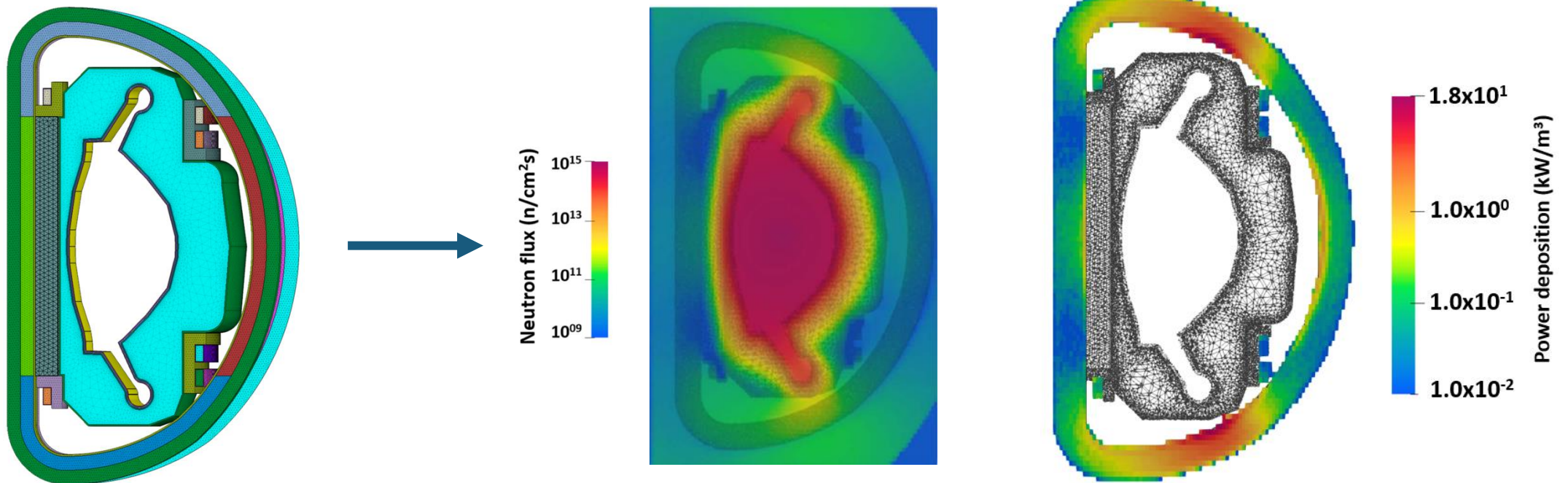
The group's goal is to develop a comprehensive modelling of irradiation effects in **HTS**.



MONTE CARLO TRANSPORT

Statistical simulation of particle trajectory and interaction distributions

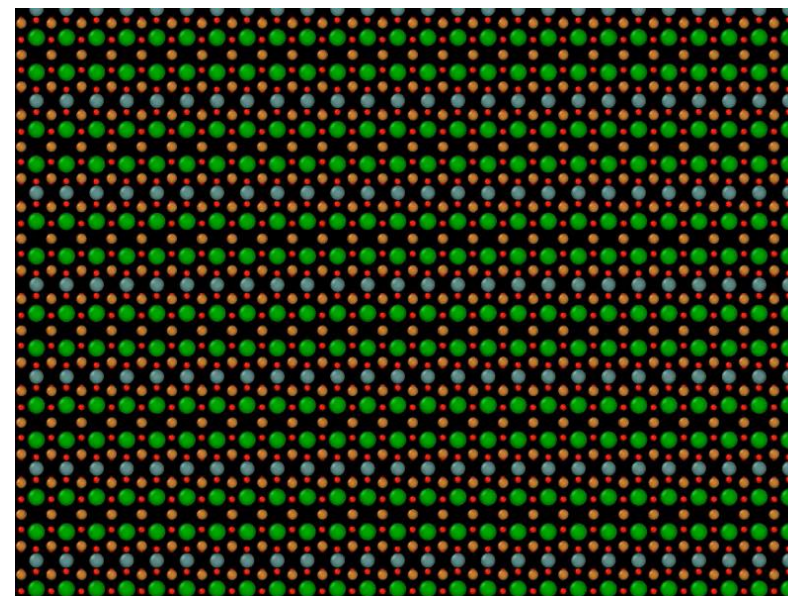
Finding **neutron spectrum, particle flux, power density deposition, dpa, PKA spectra, etc..**



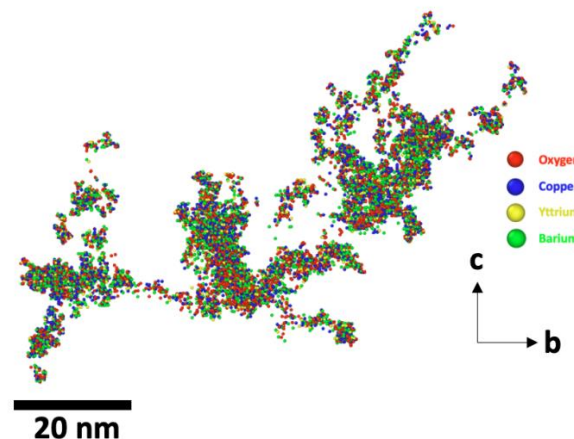
D. Torsello et al., IEEE-TAS 2024 (DOI: 10.1109/TASC.2024.3516732.)

MOLECULAR DYNAMICS

- Atom-by-atom simulation of materials
- Interactions are accounted for by means of **pseudopotentials**
- PKAs are initialised with velocities corresponding to their energy as derived from MC spectra and BCA simulations



Full defect **structure** can be obtained



BINARY COLLISION APPROXIMATION

BCA considers directly only the recoils

- More efficient tool to reproduce high energy cascades
- Reduced level of detail

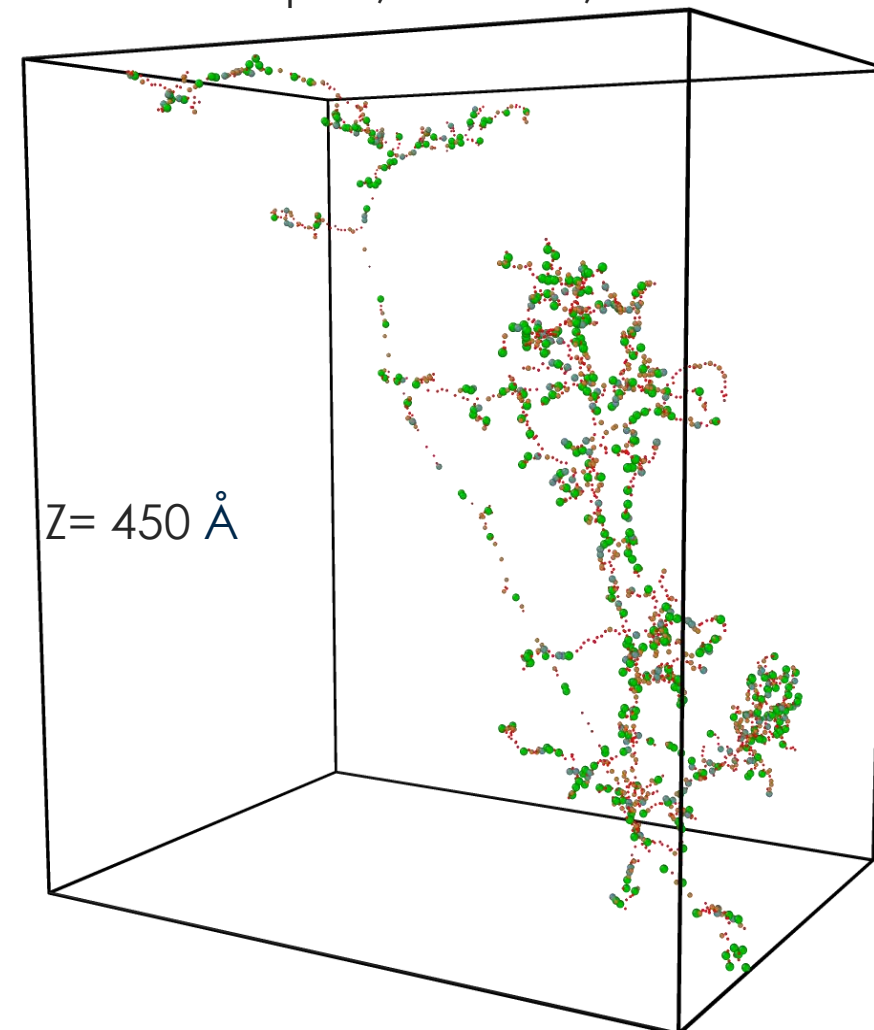
In-house code: CASWIN

- (*Pugacheva T. S. et al., NIM B 141, 99–104, 1998*)

The number of recoils with energies in the range of MD can be obtained from CASWIN:

- Each recoil can then be considered as the PKA of a lower energy cascade

Ba pka, 118 keV, 20K



MACHINE LEARNED POTENTIALS

MD simulations rely on pseudopotentials to simulate interactions between atoms

↳ A simulation can only be as accurate as the potential it uses

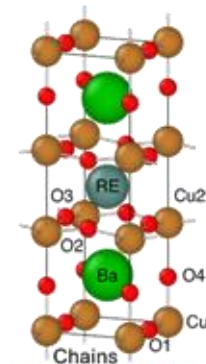
Commonly used potentials are closed formed models:

$$\phi_{\alpha\beta}(\mathbf{r}_{ij}) = \phi_{\alpha\beta}^C(\mathbf{r}_{ij}) + \phi_{\alpha\beta}^B(\mathbf{r}_{ij}) + \phi_{\alpha\beta}^{ZBL}(\mathbf{r}_{ij})$$

$$\phi_{\alpha\beta}^C(\mathbf{r}_{ij}) = \frac{q_{\alpha}q_{\beta}}{4\pi\epsilon_0 r_{ij}} \text{ (Coulomb)}$$

$$\phi_{\alpha\beta}^B(\mathbf{r}_{ij}) = A_{\alpha\beta} \exp\left(\frac{-r_{ij}}{\rho_{\alpha\beta}}\right) - \frac{C_{\alpha\beta}}{r_{ij}^6} \text{ (Buckingham)}$$

R. L. Gray et al 2022 Supercond. Sci. Technol. **35** 03501

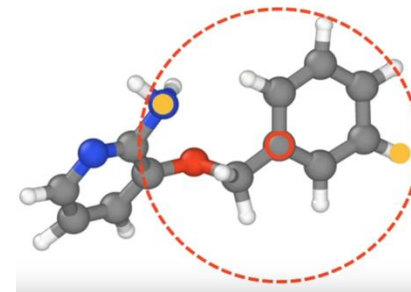


Basic idea: use DFT to build a large dataset and train a model

Con: big upfront cost to build training set

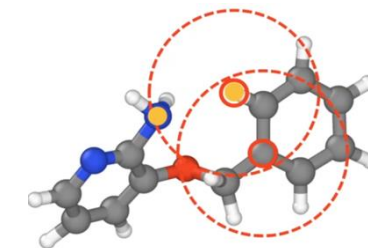
Pro: improved accuracy

Atomic Cluster Expansion (ACE)



R. Drautz 2019 *Phys. Rev. B* 99 014104

MACE (Multi-ACE)



I. Batatia et al 2022 *NeurIPS* 3511423-11436

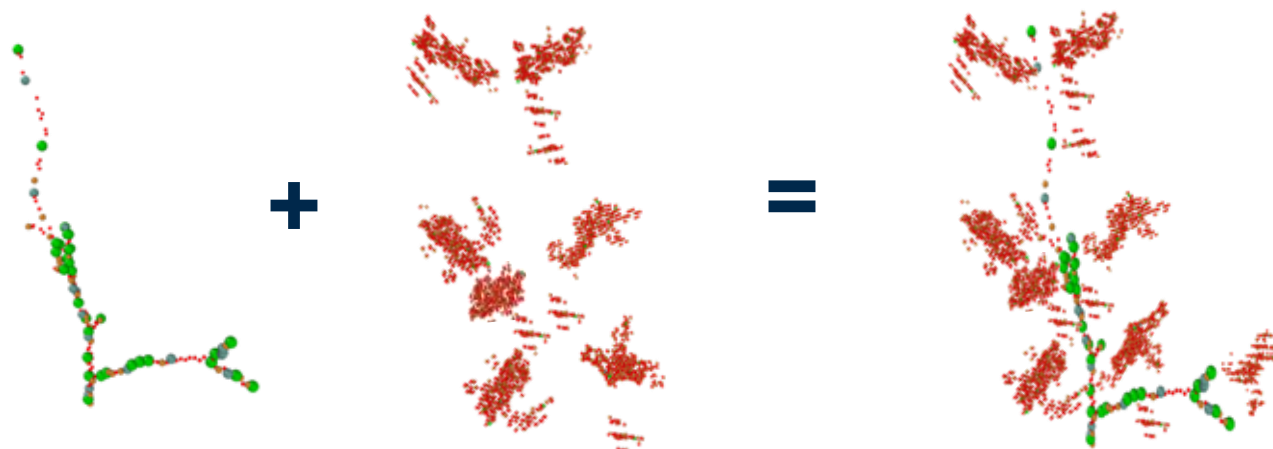
N. Di Eugenio et al., "Machine-Learned Interatomic Potentials for Structural and Defect Properties of YBaCuO", arXiv:2511.22592

A. Dickson et al., "Insights Into Radiation Damage in YBaCuO From Machine-Learned Interatomic Potentials", arXiv:2512.24430

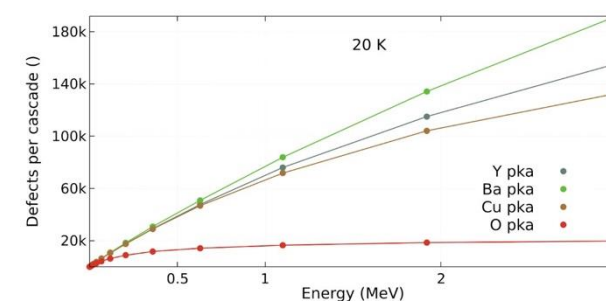
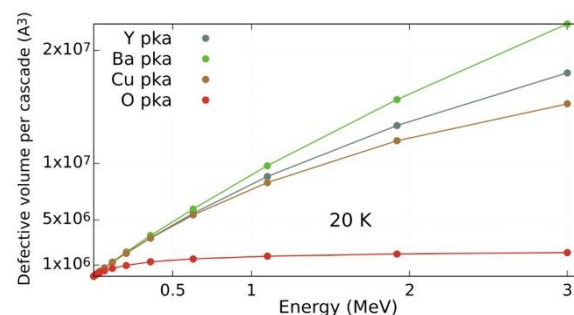
COMBINED APPROACH

Ledda et al., "Beyond dpa: an atomistic framework for a quantitative description of radiation damage in YBa₂Cu₃O₇" arXiv:2512.16249

Binary Collision Approximation +
Molecular Dynamics allows for
complete defect **morphology**
reconstruction



Transfer functions bring **microscopic**
defect information to **macroscopic**
simulation



Next step: how do these structural defects affect **superconducting performance**?

TOWARDS SUPERCONDUCTIVITY

Time Dependent Ginzburg-Landau formalism to describe superconductors

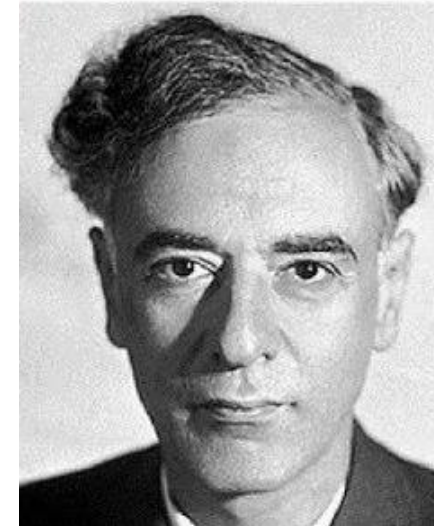
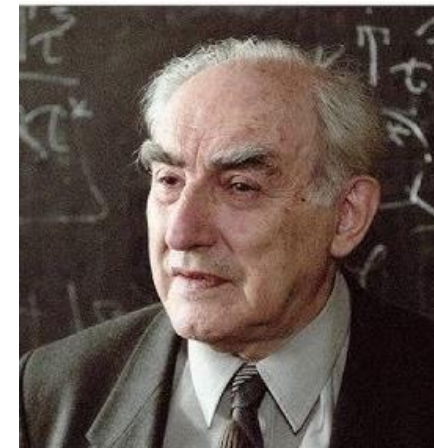
Built from GL theory of **phase transitions**, which only describes equilibrium (no dynamics)

Loosely speaking, it fits in between rigorous, microscopic descriptions and macroscopic, phenomenological models



Main strength: independent of the microscopic details of the interactions

V. Ginzburg



L. Landau

TIME-DEPENDENT GINZBURG-LANDAU MODEL

$$\frac{1}{\Gamma} \left(\frac{\partial}{\partial t} + i \frac{q}{\hbar} \mu \right) \psi = \epsilon(\mathbf{r}) \psi + u |\psi|^2 \psi - \frac{\hbar^2}{2m} \left(\nabla - i \frac{q}{\hbar} \mathbf{A} \right)^2 \psi$$

Which couples to an equation for the vector potential like $\nabla \times (\nabla \times \mathbf{A}) = \frac{4\pi}{c} [\mathbf{J}_N + \mathbf{J}_S]$

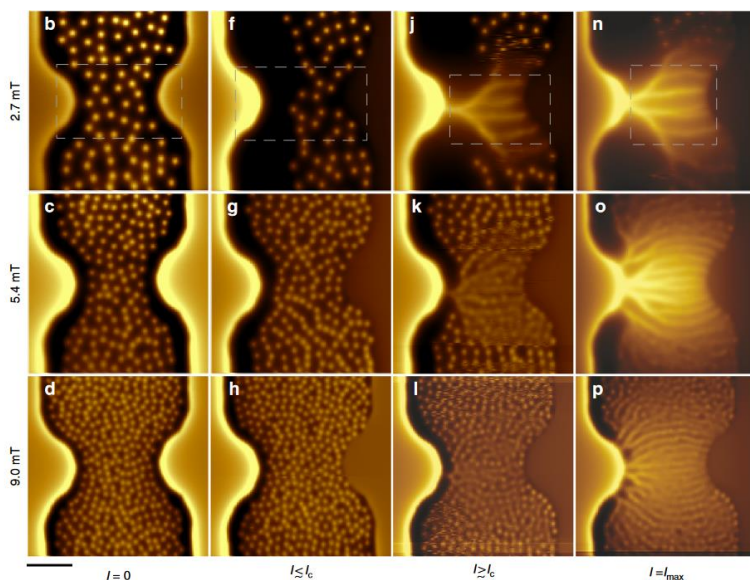
With currents

$$\mathbf{J}_N = -\sigma \left[(1/c) \partial_t \mathbf{A} + \nabla \mu \right],$$

$$\mathbf{J}_S = -\frac{e}{2m} \left[\psi^* \left(i \hbar \nabla + \frac{2e}{c} \mathbf{A} \right) \psi + \text{c.c.} \right]$$

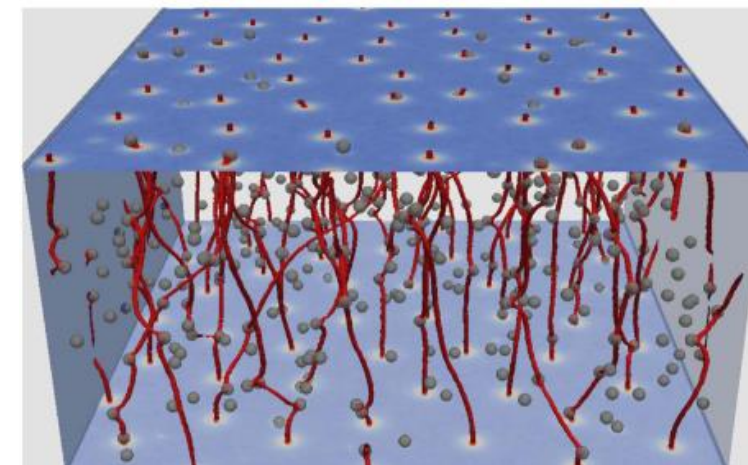
It is a system of PDEs: there are a **lot** of ways to go about the simulation

VORTICES



Main object of investigation:
superconducting vortices, i.e. filaments
of magnetic field penetrating the
superconductor

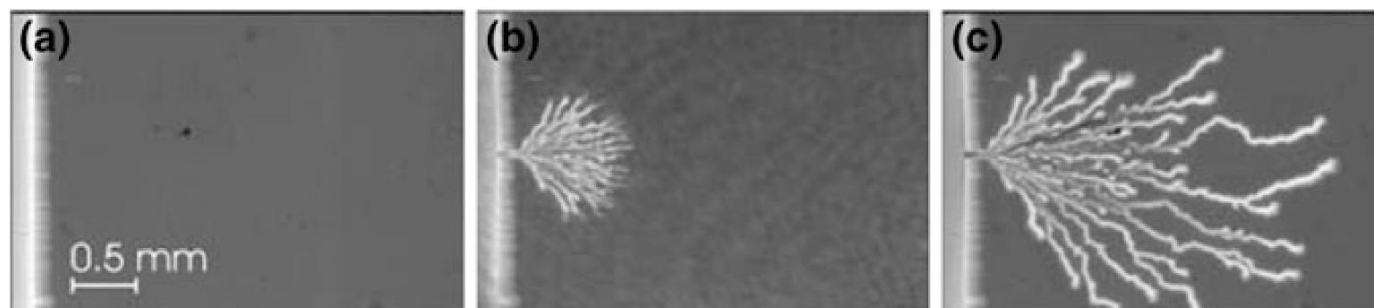
Vortices host a normal-state core, so
their motion due to Lorentz forces
dissipates energy and reduces the
material's performance



Willa et al., 2017. Strong-pinning regimes by spherical inclusions in anisotropic type-II superconductors. *Supercond. Sci. Technol.* 31, 014001.

Embon, L. et al., 2017. Imaging of super-fast dynamics and flow instabilities of superconducting vortices. *Nat Commun* 8, 85.

U. Bolz, B. Biehler, D. Schmidt, B.-U. Runge, P. Leiderer, *Europhys. Lett.* 64, 517 (2003)



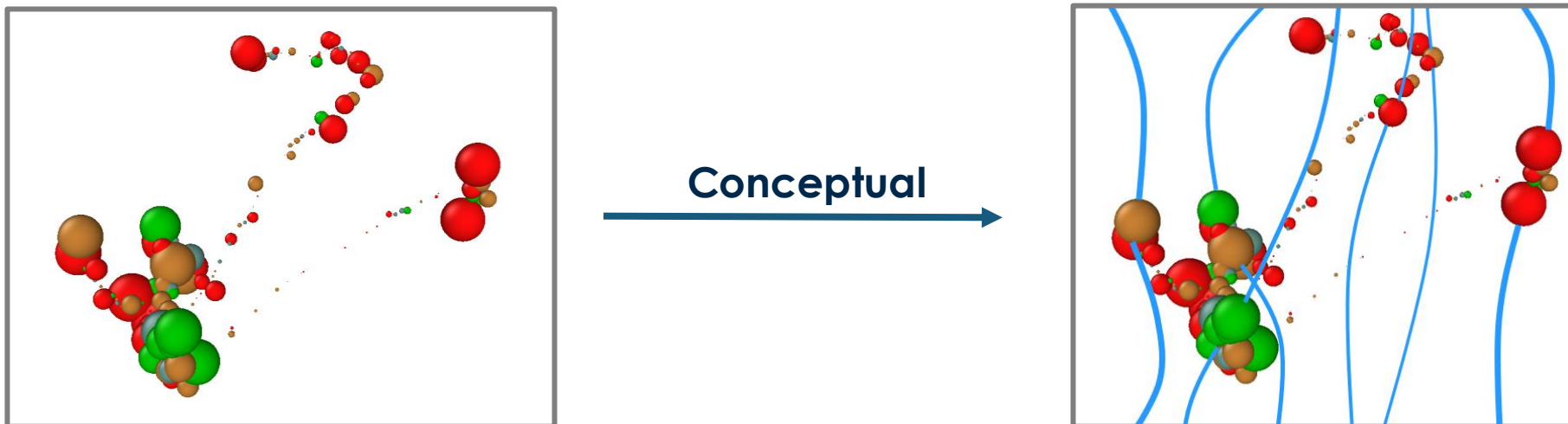
Vortices were first predicted by A. Abrikosov:
A. A. Abrikosov, "On the Magnetic Properties of Superconductors of the Second Group", *Sov. Phys. JETP* 5, 1174-1182 (1957)

NEXT STEP

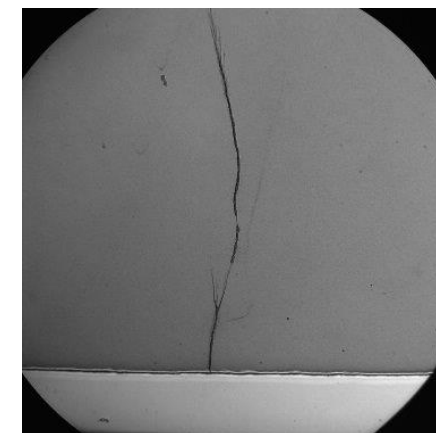
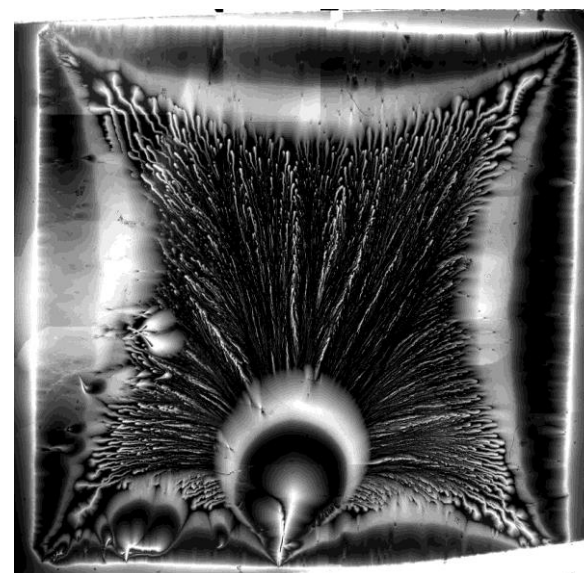
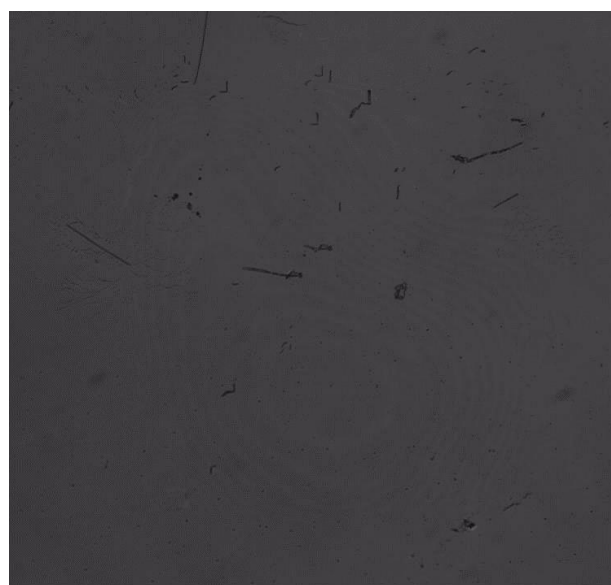
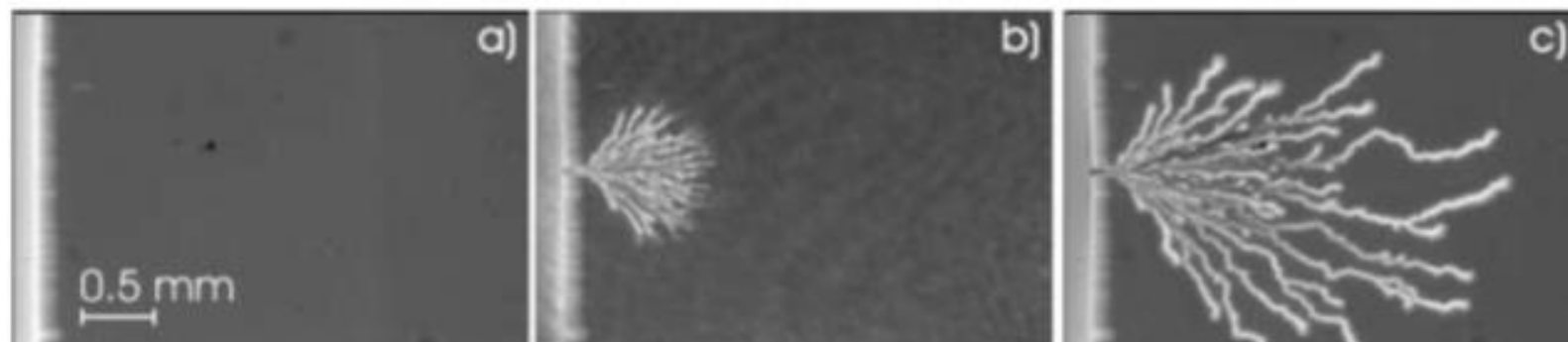
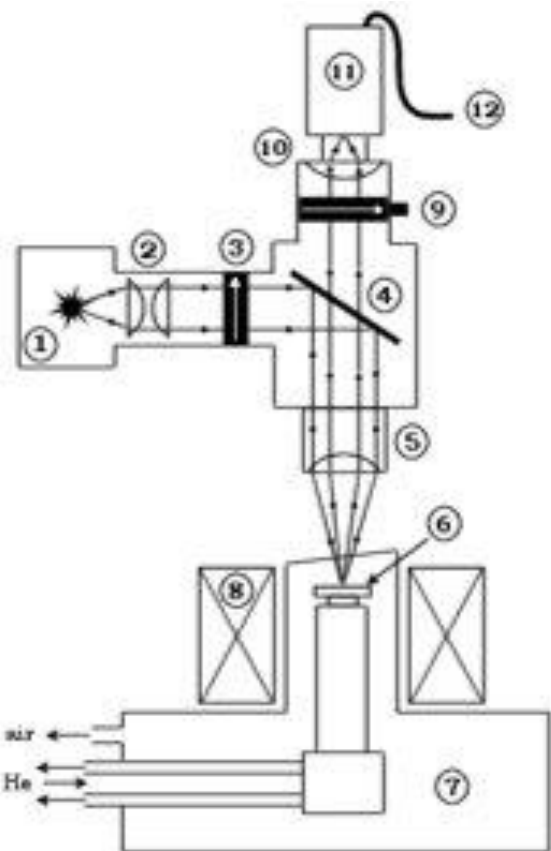
Goal: include the BCA+MD defect structures in TDGL simulation

This will allow us to characterise how they affect the superconducting state, eventually quantifying the damage that a magnet can sustain

Because of the complex and varied structure of the defects, **statistics** will need to be collected

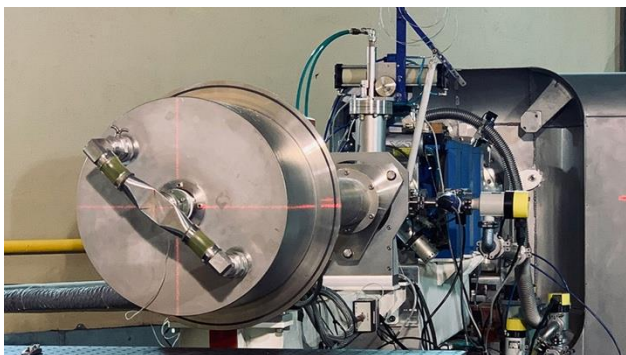
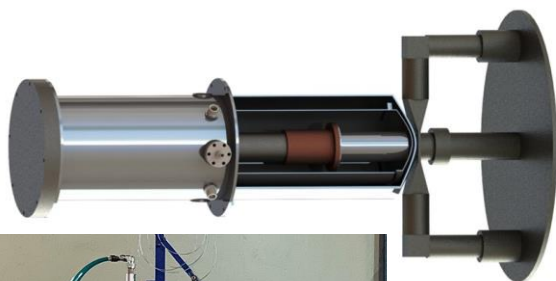


EXPERIMENTAL WORK: MAGNETO-OPTICAL IMAGING

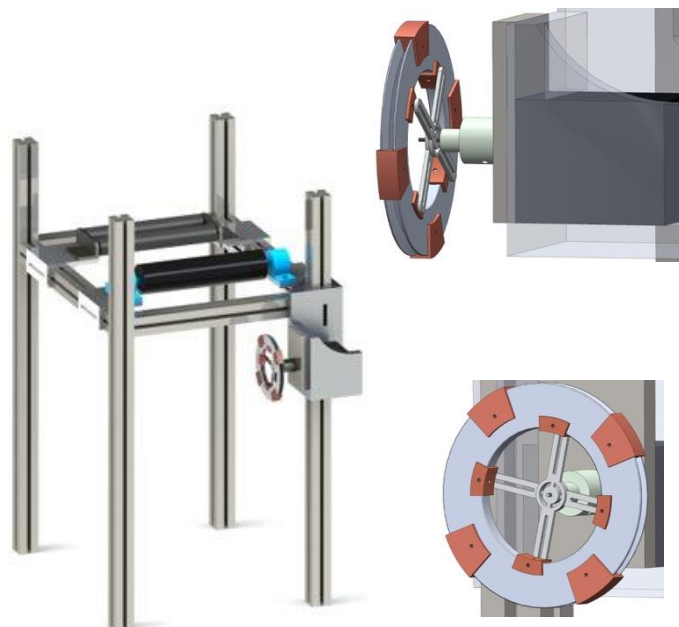


EXPERIMENTAL WORK

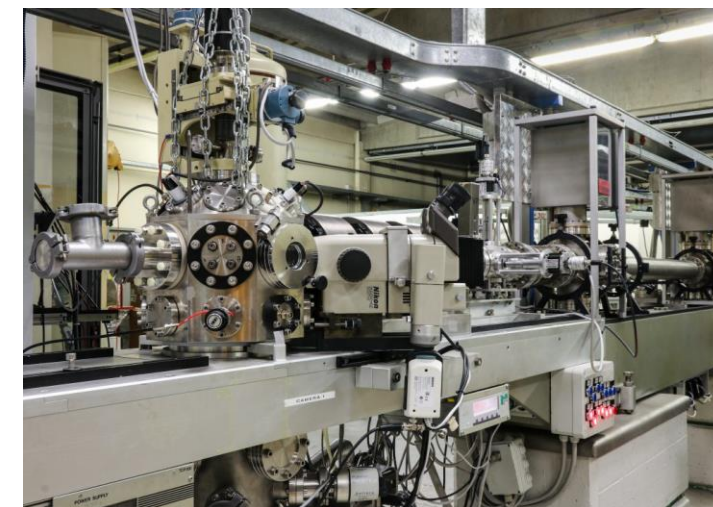
Design and development of an experimental apparatus for **cryogenic irradiation** of materials under **neutron irradiation** and **simultaneous electromagnetic** characterization at ENEA@FNG in Frascati.



Design and development of a winding machine for in-house production of **small magnets** to investigate effect of other types of stresses



Ion irradiation at INFN-LNL AN2000 for **proxy** study of damage and **validation** of the framework





THANK YOU