

# CarboEDiffSim

Simulation of Carbon electro diffusion in Iron with phase change

## MAIN PARTICIPANTS

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## OVERVIEW (keep within this page)

Starting year: 2017

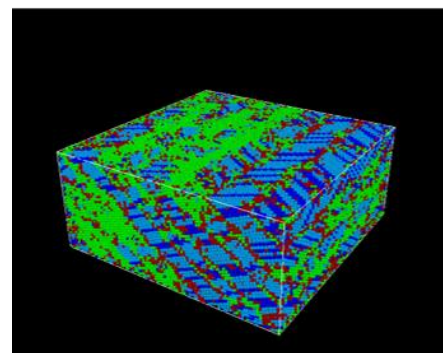
Current researchers (permanent/non-permanent): 3 person-month/year

<b>Positioning</b> <i>(Multiple selection allowed – total 100%)</i>	<b>Transportation</b>	<b>Energy</b>	<b>Eng. for Health</b>	Include partner from <input type="checkbox"/> Outside ELYT <input type="checkbox"/> Industry
				Main funding source(s) <input type="checkbox"/> Public project(s) <input type="checkbox"/> Industrial <input checked="" type="checkbox"/> Own resources
				IFS CRP/LyC project? <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No
<b>Materials and structure design</b>		50%		For main projects: Agency / year / name of project ( <i>up to 3, past projects in gray</i> )
<b>Surfaces and interfaces</b>				Estimated annual budget: None
<b>Simulation and modeling</b>		50%		
<b>Other:</b>				

### Highlights & Outstanding achievements (3-5 bullet points)

- We have made a simulation code to estimate the diffusion coefficient of carbon in iron without phase change.
- We have made a method to evaluate the phase change point by thermodynamic integration. (right figure)
- The diffusion coefficient of carbon obtained by mean square displacement is different from that obtained by the velocity of carbon induced by electrical field.
- We have a school for molecular dynamics at IFS.

### Illustration (5x5 cm<sup>2</sup> max)



## PROJECT DESCRIPTION

**Background** (10 lines max; Calibri 11)

Iron is used in a wide range of fields such as aerospace and automobiles, but it needs to be strengthened before it is used in these fields. There are many ways to strengthen it, such as work hardening, solid solution strengthening, and grain boundary strengthening. The diffusion of carbon atoms in iron is related to solid solution strengthening. Since the interstitial diffusion of carbon atoms affects the reaction rate of phase transformation of steel, the properties of iron are affected by the carbon inside the iron. Until now, the main driving force for carbon diffusion was considered to be transfer by heat, but in recent years, in the Spark Plasma Sintering method, carbon diffusion by an electric field has attracted a great deal of attention. However, although the study of carbon diffusion in iron by thermal diffusion has been widely conducted, the study of carbon diffusion under electric current has not been sufficiently conducted.

**Key scientific question** (2 lines max; Calibri 11)

Analyzing the diffusion phenomena of carbon in an electric field.  
Analyzing phase transition of iron under inclusion of carbon.

**Research method** (8 lines max; Calibri 11)

In this study, we focused on iron in the cubic lattice such as body-centered or face-centered, and performed a simulation using the molecular dynamics method to clarify the effect of the electric field on carbon diffusion inside iron. In this simulation the structural characteristics of iron are understood from the lattice constants of each temperature, and the transport characteristics of carbon at each temperature are obtained from mean square displacement. Moreover, the phase transition of iron including carbon are analyzed in detail and relation of the diffusion coefficient of carbon and each phase is obtained.

**Research students involved** (*gray color for previous years*)

Ph.D. candidates (years, institution):

- None

Master/Bachelor students (years):

- Kairi Kita (2020, IFS)

**Visits and stays** (*gray color for previous years*)

FR to JP (date, duration):

- P. Chantrenne (Feb 2020, 7 days)

JP to FR (date, duration):

- Takashi Tokumasu (Jun.-Jul. 2020, 2 months)
- Naoya Uene (Jun.-Jul. 2020, 2 months)
- Kyohei Ishikawa (Oct.-Nov. 2020, 2 months)
- Koki Nakajima (Oct.-Nov. 2020, 2 months)

## COMMUNICATIONS AND VALORIZATION

### Journal publications *(gray color for previous years)*

	Authors	Title	Journal	Vol.	pp. / ID	Year	DOI

### Conferences *(gray color for previous years)*

	Authors	Title	Conference	Date	City	Country	DOI <i>(if applicable)</i>
1	K. Kita, T. Mabuchi, P. Chantrenne, T. Tokumasu	Molecular Dynamics Study of carbon diffusion inside iron under an electric field	The 34 <sup>th</sup> Symposium on Computational Fluid Dynamics	21-23 Dec., 2020	Okinawa	Japan	<a href="https://dx.doi.org/sd.3432/0522-4530/de3c1f">https://dx.doi.org/sd.3432/0522-4530/de3c1f</a>

### Patents *(gray color for previous years)*

	Inventors	Title	PCT #	Year
1				

### Others *(gray color for previous years)*

	People	Event	Description	Date
1	Takashi Tokumasu, Patrice Chantrenne, Kairi Kita	MD School @ IFS	Teachers and students	27 <sup>th</sup> Sept. 2020