8th Postgraduate Research Symposium on Ferrous Metallurgy

Low-Activation Bainitic Steels: Design and Microstructure

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Background introduction

Challenges in Materials Science for Fusion Reactors

- Fusion reactors mimic the sun's energy production, promising a sustainable and clean energy source.
- These reactors operate under extreme conditions—high temperatures, intense neutron irradiation, and mechanical stress.
- There is a crucial need for materials that are 'low-activation', meaning they do not become long-term radioactive waste upon neutron irradiation.
- Current structural materials, such as reduced activation
 ferritic/martensitic (RAFM) steels, are under consideration
 but have limitations.



- Low-activation materials (LAMs) are defined as materials that do not activate during irradiation or quickly decay any induced radioactivity caused by transmutation from highenergy neutrons (14 MeV) in the deuterium-tritium fusion reaction, enabling safe operation and hands-on reactor maintenance ^{1,2,3,4}
- True low-activation materials weren't viable, so 'reducedactivation' steels, lacking elements causing long-lived radioactivity, were suggested. This enables safer, cheaper disposal of radioactive reactor parts post-service^{5,6,7}

Standards for the composition of low-activation steel from different countries

Chemical composition of EUROFER 97 compared to F82H mod, OPTIFER V and MANET II

	Radiologically desired	EUROFER 97	EUROFER 97	F82H mod	OPTIFER V	MANET II	
	(ppm)	specified	achieved ^a	Heat 9741 ^a	Heat 735 ^a	Heat 50804 ^a	
		(mass%)	(mass%)	(mass%)	(mass%)	(mass%)	
(A) Main a	alloying elements (mass%)						
С		0.09-0.12	0.11-0.12	0.09	0.12	0.11	
		[0.11]					
Cr		8.5-9.5 [9.0]	8.82-8.96	7.7	9.48	10.3	
W		1.0-1.2 [1.1]	1.07-1.15	1.94	0.985	-	
Mn		0.20-0.60	0.38-0.49	0.16	0.39	0.78	
		[0.40]					
V		0.15-0.25	0.18-0.20	0.16	0.245	0.2	
Ta		0.10 - 0.14	0.13-0.15	0.02	0.061	-	
		[0.12]				G	
N_2		0.015 - 0.045	0.018-0.034	0.006	0.0225	0.031	
		[0.030]					
Р		< 0.005	0.004-0.005	0.002	0.0035	0.003	
S		< 0.005	0.003-0.004	0.002	0.0025	0.004	
в		< 0.001	0.0005-0.0009	0.0002	0.0002	0.0073	
O_2		< 0.01	0.0013-0.0018	0.01	0.006	c	
(B) Radiol	ogiocally undesired elements (mass?	6 and u g/g = ppm)					
Nb	<0.01	[<10]	2-7	1	70	1400	
Mo	<1	[<50]	10-32	30	50	6100	
Ni	<10	[<50]	70-280 ^b	200	50	6800	
Cu	<10	[<50]	15-220 ^b	100	50	100	
Al	<1	[<100]	60-90	30	70	40	
Ti	<200	<100	50-90	100	70		
Si	<400	<500	400-700	1100	60	1900	
Co	<10	[<50]	30-70	50			

Nb < 0.001, Mo < 0.005, Ni < 0.005, Cu < 0.005, Al < 0.01, Ti < 0.01, Si < 0.05, Co < 0.005.

References:

^{1.}Conn, R.W., Bloom, E.E., Davis, J.W., Gold, R.E., Little, R., Schultz, K.R., et al. (1984). 'Report on low activation materials for fusion applications.'

^{2.}Butterworth, G.W., & Jarvis, O.N. (1984). 'Comparison of transmutation and activation effects in five ferritic alloys and AISI 316 stainless steel.'

^{3.}Ghoniem, N.M., Shabaik, A., & Youssef, M.Z. (1984). 'Development of low activation vanadium steel for fusion applications.' In Davis, J.W. & Michel, D.J. (Eds.), Proceedings of the Topical Conference on Ferritic Steels for Use in Nuclear Energy Technologies.

^{4.}Klueh, R.L., & Bloom, E.E. (1985). 'The development of ferritic steels for fast induced-radioactivity decay for fusion reactor applications.'

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^{6.}Dulieu, D., Tupholme, K.W., & Butterworth, G.J. (1986). 'Development of low-activation martensitic stainless steels.'

^{7.} Tamura, M., Hayakawa, H., Tanimura, M., Hishinuma, A., & Kondo, T. (1986). 'Development of potential low activation ferritic and austenitic steels.'

-History of Low-activation Steels

Early Developments

martensitic steels.

•1960s-1970s: Initiatives in the US and Europe to reduce nuclear reactor environmental impact.

•Focus: Developing FM steels with 8-9% chromium (Cr).

•Substitutions: Mo and Nb replaced with W and Ta to reduce long-lived isotopes.

•Impurities Control: Tight limits on elements like P, S, and Si.

Development in the United States

•**1980s**: Oak Ridge National Laboratory developed 9Cr-2WVTa (T91) steel.

•Features: Maintains structural integrity in high neutron flux, with a DBTT increase of only 32°C after irradiation.
•Performance: Superior tensile strength and impact toughness compared to other reduced activation



The transition temperature as a function of fluence for 9Cr-2WV and 9Cr-2WVTa steels irradiated at 365 $^{\circ}\rm C$ in the FFTF, after Klueh .

—History of Low-activation Steels

Key Developments in Asia

•Japan: Developed F82H steel with minimal DBTT shift and high resistance to irradiation-induced embrittlement.

•China: Developed China Low-activation Martensitic (CLAM) steel for projects like CFETR and ITER, known for excellent irradiation resistance and high thermal conductivity.

European Contributions

•EUROFER: Developed by the European Fusion Development Agreement (EFDA), known for its excellent mechanical properties and reduced activation characteristics.

•**Performance**: Demonstrates impressive creep strength and maintains good tensile properties and microhardness under various conditions.



Larson–Miller-Plot for EUROFER 97 bar and plate material with different heat treatments in comparison with OPTIFER developmental alloy, F82H mod. and ODS-EUROFER, after R Lindau.

---Limitations of Current LAFM Steels

Insufficient High-Temperature Creep Strength

•Limitation: Traditional low-activation ferritic/martensitic (FM) steels struggle at temperatures above 550°C.

•Impact: Poor high-temperature performance limits their use in nuclear reactors.

Examples of Weaknesses

•Creep Rupture Life:

- **550°C**: Significant decrease under 180-220 MPa stresses.
- **Example**: Reduction from 202 hours to 111 hours after thermal aging (550°C for 4000 hours).

•Minimum Creep Rate:

• **Increase**: From $3.61 \times 10^{-4} \cdot s^{-1}$ to $6.84 \times 10^{-4} \cdot s^{-1}$ post

aging.



The rupture life and minimum creep rate of CLAM steel after different aging time, after Wang, W.

----Limitations of Current LAFM Steels

Low-Temperature Irradiation Embrittlement

Limitation:

•Low-activation steels undergo significant embrittlement when irradiated at low temperatures (around 300°C), compromising structural integrity in cold environments.

Impact:

•Increased risk of material fracture under low-temperature conditions limits potential applications in such environments.

Examples of Weaknesses

Temperature-Dependent Embrittlement:

•Below 350°C: All low-activation ferritic martensitic

(LAFM) steels exhibited significant radiation-induced embrittlement.

•**Impact**: DBTT increases significantly, indicating substantial embrittlement and increased fracture risk.



Ductile-to-brittle transition temperature vs. irradiation temperature and (b) Irradiation-induced shifts of ductile-to-brittle transition temperature vs. irradiation temperature, after Gaganidze, E. et al.

-----Limitations of Current LAFM Steels Low-Temperature Irradiation Hardening

Limitation:

•Low-activation steels exhibit significant hardening when irradiated, particularly at low temperatures around 300°C to 350°C. **Impact:**

•The mechanical properties, such as yield strength and ductility, degrade significantly, restricting their application scope and lifespan in nuclear fields.

Examples of Weaknesses

Increased Yield Strength and Brittleness:

•300-350°C Irradiation: Low-activation steel EUROFER97, when irradiated at doses between 0-20 displacements per atom (dpa), shows a significant increase in yield strength ($\Delta R_{p0.2}$), leading to increased brittleness. •Impact: Yield strength increases sharply with irradiation dose and eventually saturates.



Literature review ——Why design bainitic steel?

Enhanced Creep Resistance: Bainitic steels exhibit superior creep resistance compared to martensitic or ferritic steels, crucial for maintaining structural integrity under high temperatures and long-term stresses^{1,2,3}.

Sustained Strength: Offers improved mechanical properties and sustained strength at high temperatures, essential for applications in nuclear and energy sectors^{4,5}.

However, bainite steels contain some Radiologiocally undesired elements!



References:

1. Puype et al., 2018. "Design of Reduced Activation Ferritic/Martensitic Steels with Improved Creep Resistance by Thermodynamic Modelling."

2.Shankar et al., 2016. "Influence of Varying W and Ta on Low Cycle Fatigue and Creep-Fatigue Interaction Behavior of Reduced Activation Ferritic/Martensitic Steels."

3.Kohyama et al., "Irradiation creep behavior of low activation steels in FFTF/MOTA."

4.Liu et al., 2023. "Research on thermal creep behavior of Chinese low-activation ferritic/martensitic steel."

5. Ahiale et al., 2022. "Low-Cycle Fatigue Behavior of Reduced Activation Ferritic-Martensitic Steel at Elevated Temperatures."

2. Generating High Creep-Resistant Low-Activation Bainitic Steel Compositions Using Multi-Objective Optimisation Genetic Algorithm



Dataset Description

- ➤ Total number of columns: 25 columns.
- ➤ Number of independent variables (factors): 21.
- Number of dependent variables (outcomes): 4, which is "Yield strength, Tensile strength, Elongation ,Time to rupture".

Variable Name	Min	Max	Mean	Median
С	0.08	0.25	0.134939	0.13
Si	0.03	0.86	0.324738	0.3
Mn	0.38	55	1.292972	0.5
Р	0	0.029	0.012561	0.012
S	0	0.022	0.007311	0.007
Ni	0	0.9	0.135541	0.047
Мо	0	1.22	0.653123	0.92
Ν	0.002	0.06	0.015904	0.0115
Cr	0	12.9	5.859299	8.6
W	0	1.52	0.377657	0
V	0	0.3	0.077949	0
Со	0	0.15	0.007933	0
Та	0	0.2	0.027258	0
Cu	0	0.16	0.047578	0.03
Al	0	0.042	0.009048	0.005
yield strength	249	875	472.3824	420
Tensile strength	430	1031	654.0248	589
elongation	13	38	26.24357	29
stress	18	530	171.3188	137
temperature	450	700	564.5075	550
Time to rupture	0.1	172961	15265.58	3787

Range of Independent and Dependent Variables

Optimisation and selection of the predictive model



Optimisation and selection of the predictive model



- The ensemble methods, specifically GBDT and XGBoost, outperform other models in predicting creep rupture time.
- > Random Forest, while not as effective as GBDT and XGBoost, still demonstrates good predictive ability.
- Linear Regression, Deep Learning, and MLP models are not suitable for this task, as indicated by their low R^2 values and high error metrics.
- The choice of model for predicting creep rupture time should favor ensemble methods, which seem to handle the underlying data complexity better.

Optimisation and selection of the predictive model



Reverse generation algorithm ——Genetic algorithm



Key parameters of the genetic algorithm Fitness=1 / ((prediction - target) ** 2 + 1) population_size = 100 generations = 100 mutation_rate = 0.8 num_best_individuals = 10

Reverse generation algorithm ——Determination of constraints



- Set the constraints for the genetic algorithm according to the literature: test temperature 650°C, stress 70Mpa, rupture life 10000 hours. This is far above the current European standards.
- At the same time, limit the content of radiologically undesired elements: Nb < 0.001, Mo < 0.005, Ni < 0.005, Cu < 0.005, Al < 0.01, Ti < 0.01, Si < 0.05, Co < 0.005.

Note: Both axes are on a logarithmic scale

a)

Reverse generation algorithm

——The results of the reverse generation

The final composition combinations

Alloy Number	С	Si	Mn	Ni	Мо	Cr	W	V	Со	Та	Cu	Al	Fe	Prediction
1	0.09	0.017	0.22	0	0.001	8.29	0.79	0.09	0	0.18	0.004	0.006	90.312	10001.08492
2	0.12	0.003	0.46	0.003	0.002	4.79	0.62	0.05	0.004	0.04	0.002	0.003	93.903	9996.49585
3	0.15	0.031	0.34	0.002	0.003	5.71	0.82	0.11	0.002	0.2	0.001	0	92.631	10002.62861
4	0.1	0.014	0.49	0.002	0.002	4.13	0.77	0.16	0.004	0.06	0.004	0.004	94.26	10002.97521
5	0.11	0.03	0.66	0.001	0.004	2.82	0.91	0.08	0.003	0.13	0	0.005	95.247	9999.462526
6	0.11	0.02	0.49	0.004	0.004	3.56	0.85	0.03	0.002	0.09	0.002	0.003	94.835	10000.15292
7	0.13	0.017	0.45	0.002	0.001	8.74	0.82	0.04	0.001	0.07	0.003	0.003	89.723	10001.61434
8	0.1	0.033	0.56	0.004	0.002	2.4	0.4	0.08	0.002	0.13	0	0.008	96.281	9999.858244
9	0.09	0.027	0.38	0.001	0.002	9.19	0.84	0.02	0.001	0.08	0.001	0.007	89.361	10000.43292
10	0.12	0.025	0.26	0.003	0.002	3.11	0.91	0.15	0.004	0.18	0.001	0.008	95.227	10000.6239





Fitness Evolution over Generations

Reverse generation algorithm

——Elemental Content: Original vs. Generated Histograms



3. Modelling Radiation hardening

Research Background

—The concept of radiation hardening

•Radiation Hardening:

•Definition: A phenomenon where the material's microstructure changes under high-energy radiation (e.g., neutron irradiation), leading to increased yield strength and brittleness.

•Causes: Displacement damage and radiation-induced defects (e.g., vacancies and interstitial atoms) accumulate, hindering dislocation movement.

•Effects:

- •Increased yield strength
- •Higher susceptibility to brittle fracture and fatigue failure



Research Background ——Why need radiation hardening model?

•Factors Influencing Hardening:

•Chemical composition of the steel

•Irradiation variables: dose, dose rate, and temperature

•Challenges in Study:

•Complex mechanisms

•Traditional statistical methods are insufficient for accurate analysis

•Importance of Prediction Models:

•Traditional experiments are time-consuming, costly, and risky.

•Developing accurate radiation hardening prediction models is crucial for advancing nuclear reactor materials.

Dataset description

Based on the collected data, the dataset consists of 1866 entries with the following columns: Independent Variables (Chemical Composition and Radiation Conditions): **Chemical Composition**** (22 columns) **Radiation Conditions**** (4 columns): - T_{irr} (°C) (Irradiation Temperature) - Irr_{Dpa} (Irradiation Damage) - He_{dpa} (Helium Damage) - T_{Test} (°C) (Testing Temperature) Dependent Variable** (1 column):

- Yield Stress	s (MPa)
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Variables	Mean	Standard Deviation	Maximum	Minimum
С	0.09719	0.01307	0.2	0.0092
Cr	8.37662	0.83372	12	2.25
W	1.49473	0.77203	3	0
Мо	0.14963	0.35411	1	0
Та	0.06326	0.10049	0.54	0
V	0.18353	0.05377	0.3	0
Si	0.05564	0.05114	0.37	0
Mn	0.15650	0.20740	1.13	0
Ν	0.00268	0.00800	0.06	0
Al	0.00111	0.00413	0.054	0
As	0.00002	0.00028	0.005	0
В	0.00074	0.00142	0.0085	0
Со	0.00015	0.00088	0.01	0
Cu	0.00056	0.00308	0.035	0
Nb	0.01594	0.10509	1.6	0
Ni	0.05615	0.30222	2	0
0	0.00015	0.00103	0.009	0
Р	0.00136	0.00140	0.007	0
Pb	0.00002	0.00028	0.005	0
S	0.00123	0.00116	0.005	0
Ti	0.00977	0.04504	0.25	0
Zr	0.00023	0.00325	0.059	0
T _{irr} (°C)	410.064	182.33523	925	273
Dose (dpa)	3.85271	10.37125	90	0
He (appm)	55.99097	577.83253	6315	0
T _{test} (°C)	553.94598	208.85996	996	123
Yield Stress (MPa)	544.03315	189.58747	1539	117

Distribution Plot of Variables



Box Plot of Variables



Hyperparameter Optimisation Method

Three models were selected: Gradient Boosting Decision Trees (GBDT), XGBoost, and Random Forests (RF). I manually chose the three most important hyperparameters for each model. For XGBoost, the chosen hyperparameters were:

- **n_estimators**: 5000, 10000, 15000, 20000
- **max_depth**: 5 to 20 (increments of 1)
- **eta**: 0.00035 to 0.0015 (5 evenly spaced values) For GBDT, the chosen hyperparameters were:
- **n_estimators**: 5000, 10000, 15000, 20000
- learning_rate: 0.0001 to 0.001 (5 evenly spaced values)
- **max_depth**: 5 to 12 (increments of 1)
- For Random Forests, the chosen hyperparameters were:
- n_estimators: 50 to 1000 (increments of 50)
- **max_features**: 1 to 17 (increments of 1)
- **max_depth**: 5 to 20 (increments of 1)

The formulas for these metrics are as follows:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \overline{y})^{2}}$$
$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}$$

$$PCC = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{\left[n\sum x^2 - (\sum x)^2\right]\left[n\sum y^2 - (\sum y)^2\right]}}$$

Where

- y_i : Actual value of the i-th observation.
- \hat{y}_i : Predicted value of the i-th observation,
- \overline{y} : Mean of the actual values.
- **x** : First set of data,
- **y** : Second set of data

Hyperparameter Optimisation for GBDT



Hyperparameter Optimisation for XGBoost



Hyperparameter Optimisation for RF



Results of Hyperparameter Optimisation

As for GBDT, the following hyperparameter ranges are identified as optimal: 1. n_estimators: **12500 to 15000** (0.5 to 0.75 in the proportion)

2. learning_rate: **0.0004 to 0.0008** (0.25 to 0.50 in the proportion)

3. max_depth: 8 to 11 (0.5 to 0.75 in the proportion)

As for RF, the following hyperparameter ranges are identified as optimal:

1. n_estimators: **125 to 250** (0.5 to 0.75 in the proportion)

2. max_features: 9 to 13 (0.50 to 0.75 in the proportion)

3. max_depth: **10 to 15** (0.50 to 0.75 in the proportion)

As for XGBoost, This **lack of overlapping regions** suggests that the XGBoost model is **overfitting** to the training data and does not generalise well to the test data. The model's high performance on the training set does not translate to the test set, indicating poor generalisation ability and the presence of overfitting. Therefore, XGBoost is **not suitable for this dataset**.

Model training and selection



•Both models perform well, but GBDT slightly outperforms RF.

•Therefore, GBDT is selected as the predictive model for radiation hardening.

Feature Importance Analysis



•Tantalum (Ta): Highest importance, most significant impact on yield stress.

•Tungsten (W): High importance, notable influence.

•Sulphur (S): Significant impact.

Chromium (Cr) and Niobium (Nb): Moderate importance.
Nickel (Ni), Carbon (C), Silicon (Si), and Phosphorus (P): Lower importance, smaller impact.

Importance of Radiation Condition Variables:

•**Test Temperature** (T_{test}): Highest importance, most significant impact on yield stress.

•Irradiation Dose (Dose, dpa): High importance, significant effect.

•Irradiation Temperature (Tirr): Moderate importance.

Validation of the Model



Irradiation Temperature and Test Temperature (°C)









Comparing Radiation Hardening Behavior of Different Steels Using Models



Analyzing the Impact of Different Elements on Radiation Hardening Behavior



From the polar plot for W:

•Temperature Range (0°C to 375°C):

- **General Trend:** Noticeable radiation hardening across the entire range.
- 0°C to 125°C: Radiation hardening is relatively mild.
- 125°C to 250°C:
 - For W content between 0-2 wt.%, hardening intensity increases.
 - For W content between 2-3 wt.%, hardening intensity decreases as W content increases.

• 250°C to 375°C:

- Radiation hardening further intensifies.
- Peak Hardening: Around 315°C.
 - W Content <0.5 wt.% or 1.5-2.5 wt.%: Maximum hardening, reaching approximately 700 MPa.

•Above 375°C:

• **Trend:** Rapid decrease in radiation hardening.

Analyzing the Impact of Different Elements on Radiation Hardening Behavior

From the polar plot for Cr:

•Temperature Range (0°C to 375°C):

- **General Trend:** Significant radiation hardening across all Cr content ranges, with hardening levels higher than those of W.
- 0°C to 125°C:
 - Noticeable radiation hardening at Cr content levels between 6-8 wt.%, reaching around 500 MPa.

• 125°C to 250°C:

- Hardening further intensifies, especially for Cr content between 0-3 wt.%, achieving approximately 600 MPa.
- For Cr content between 4-8 wt.%, hardening levels are relatively lower.
- 250°C to 315°C:
 - Radiation hardening continues to increase, peaking around 315°C.
 - Peak hardening of approximately 750 MPa is observed at Cr content levels between 0-0.5 wt.% and 6-8 wt.%.

•Above 375°C:

• Trend: Rapid reduction in radiation hardening.



Analyzing the Impact of Different Elements on Radiation Hardening Behavior



From the polar plot for Ta:

•General Observation: Radiation hardening for Ta is significantly lower than that for W and Cr across the entire temperature range.

•0°C to 125°C:

• No significant radiation hardening observed.

•125°C to 250°C:

- Rapid increase in radiation hardening.
- Peak hardening of approximately 650 MPa at Ta content between 0-0.2 wt.%.
- Hardening significantly decreases for Ta content between 0.2-0.5 wt.%.
- Slight increase in hardening observed for Ta content between 0.5-0.6 wt.%.

•250°C to 375°C:

- Hardening decreases overall.
- At 315°C, an increase in hardening to around 400 MPa is observed for Ta content between 0.3-0.4 wt.%.

•Above 375°C:

• Rapid decrease in radiation hardening.

Thanks for listening