PREDICTION OF MECHANICAL, ELECTRIC, AND THERMAL PROPERTIES OF COPPER ALLOYS BASED ON COMPOSITION AND PROCESSING USING MACHINE LEARNING

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INTRODUCTION

Problems

- The application of **leadframes** requires a complex set of specifications, including **high strength**, **high conductivity**, and **low thermal expansion coefficient** to ensure optimal performance.
- **Discovering copper materials** that achieve this combination of properties through **experimental method** involves **significant costs** and is **time-consuming**.

Objective

Develop ML models for **predicting** and **reverse-predicting** the tensile strength, electrical conductivity, and thermal expansion coefficient of copper alloys based on their chemical composition and processing methods and to **assess the performance** of these models in **selecting optimal copper alloy materials**.

METHODOLOGY

Machine Learning Modelling

Dataset → Model Design → Model Training → Parameter Optimization → Model Design

* Consisting of property prediction model (C2P) and their reserve prediction model (P2C)

Machine Learning Design System (MLDS)

Target Property → P2C → C2P → Predicted Property

Target Property → Error < e ← Predicted Property

Error < e: No → P2C; Yes → Alloy Design

RESULT

- **From the six trained models** (KNN, RF, ExtraTrees, Catboost, XGB, and BPNN), the two **best C2P and P2C** models obtained are **BPNN** and **XGB** as shown in Figure 1.
- **MLDS XGB** shows **lower fluctuations** compared to **MLDS BPNN** and **P2C BPNN** in providing recommendations for copper alloy composition and processing, spesifically referencing **C41300** material as shown in Figure 2.
- **MLDS XGB** can be used to **recommend new copper alloys** for leadframe applications that are **in line** with the **literature** as shown in Table 1.

Fig 1. The performance of the best C2P and P2C models

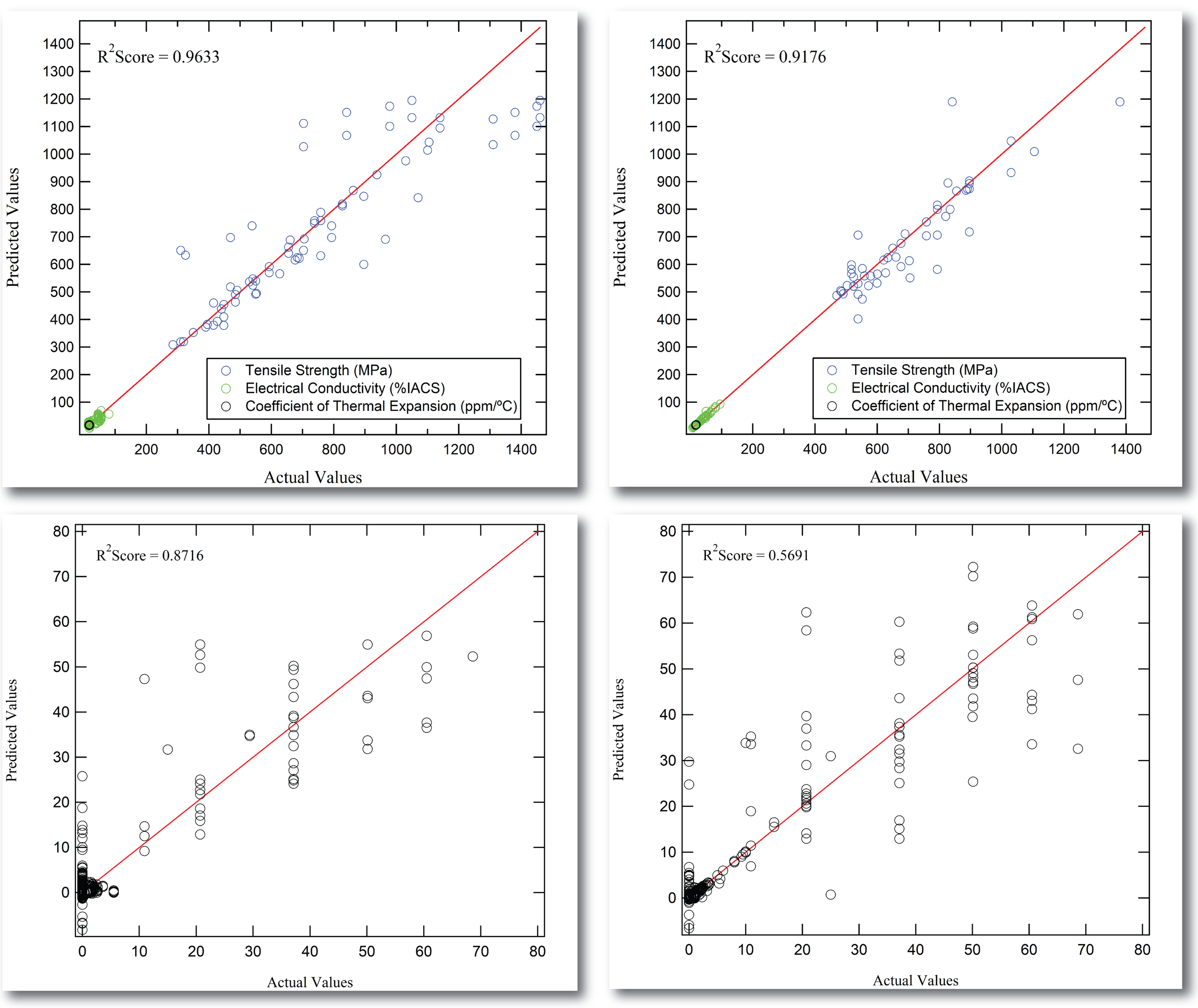

Fig 2. Main elements (Zn and Sn) of alloy designed by MLDS and P2C models

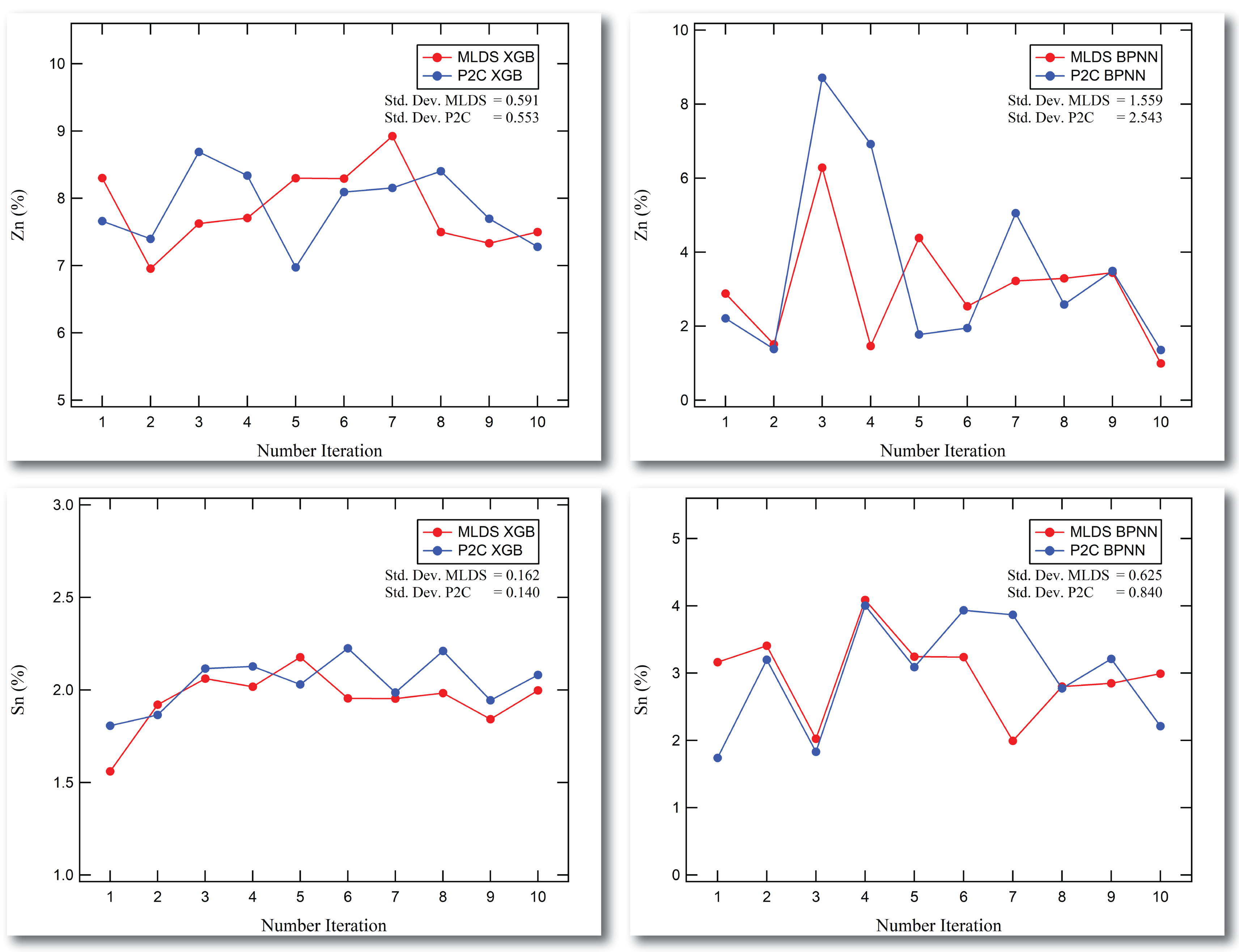

Table 1. Design Result and Verification

Target	MLDS Result	Experimental Design	Experimental Result
575 MPa 85% IACS 17 ppm/°C	● Cu-0.21Fe-0.16Zr-0.52Cr-0.03Ti-0.04Ag (C) ● Solution treatment, 45% CR, and aging (P)	● Cu-0.15Zr-0.5Cr-0.1Ag (C) ● Solution treatment, 80% CR, and aging (P)	570 MPa 86% IACS

CONCLUSION

BPNN and XGB are the **two best models** for C2P and P2C, but the **performance of MLDS XGB** in recommending copper alloy composition and processing is **significantly better**.