Materials Science Analysis & Prediction System

AI-Powered Solution for Material Property Prediction & Fracture Analysis

Machine Learning | Deep Learning | Computer Vision | Generative AI

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Project Overview

🎯 The Challenge

In automotive and manufacturing industries, understanding material failure modes is critical for:

- Product Safety – Preventing catastrophic failures
- Quality Control – Ensuring material specifications
- Cost Reduction – Minimizing expensive lab testing
- Process Optimization – Fine-tuning heat treatment

💡 Our Solution

An end-to-end AI system that combines:

- Predictive Analytics – Material property prediction
- Computer Vision – SEM fracture image analysis
- Generative AI – Intelligent document Q&A
- Web Applications – User-friendly interfaces

📊

Exploratory Data Analysis

Statistical insights from 385,000 material samples

🤖

Machine Learning

Predict ductility & brittleness properties

🧠

Deep Learning

SEM fracture image classification

✨

Generative AI (RAG)

AI-powered Q&A for ISO/DIN standards

Datasets Overview

Axle Test Data

Size: 385,000 samples
Material: 4Cr13 Stainless Steel
Features: 24 variables

Chemical Composition:
· C, Si, Mn, P, S (%)
· Cr, Ni, Cu, Mo (%)

Mechanical Properties:
· HV10 Hardness values
· Bending Force (N)

Heat Treatment:
· Hardening temperature
· Tempering conditions

Target Variables:
· Ductility %
· Brittleness %

SEM Images

Type: Fracture Surface Images
Format: 16,268 TIFF files
Size: -30 GB total

Image Characteristics:
· High-resolution microscopy
· Grayscale format
· Various magnifications

Classification Classes:
· Ductile (Dimples)
  – Rounded cup-like structures
  – Indicates plastic deformation

· Brittle (Cleavages)
  – Flat faceted surfaces
  – Indicates sudden failure

Purpose: Visual fracture analysis

Technical Documents

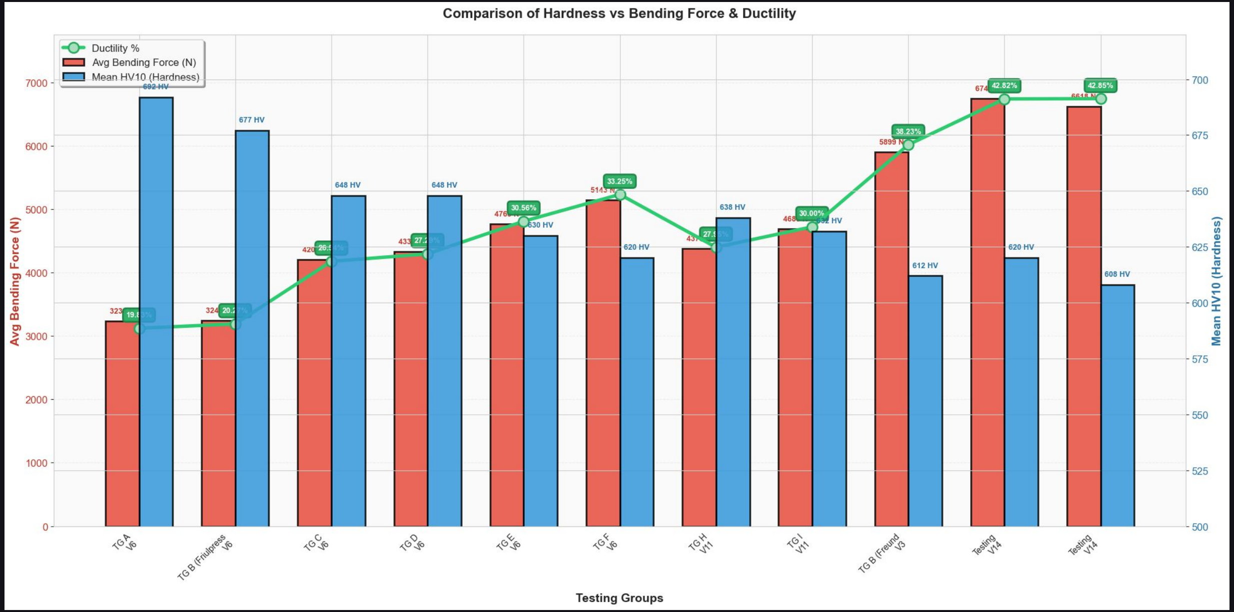
Content: 50+ PDF Documents
Focus: ISO/DIN Standards

Topics Covered:
· Metallography procedures
· Hardness testing standards
· Material specifications
· SEM analysis guidelines

Standards Included:
· ISO 643 – Grain size
· ISO 6507 – Vickers hardness
· ISO 6506 – Brinell hardness
· ISO 6892 – Tensile testing
· DIN 50190 – Hardness depth

RAG System:
· 13,400+ text chunks
· Semantic search enabled
· AI-powered Q&A

Exploratory Data Analysis



Key Insights

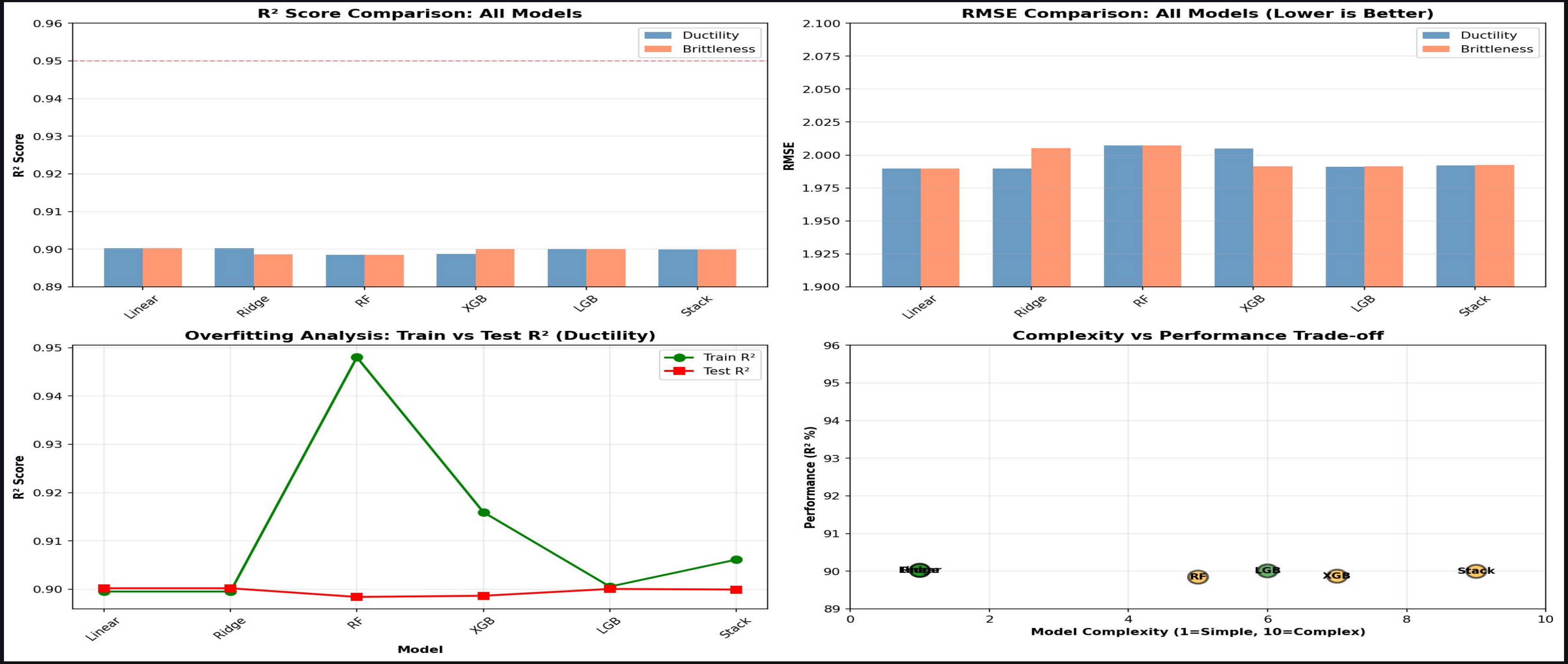
📊 Dataset Quality
- 385,000 clean samples
- Zero missing values
- No duplicate records

📈 Target Distribution
- Ductility: 15% – 47%
- Mean: 27.27%
- Std Dev: ±6.29%

🔗 Top Correlations
- Bending Force → Ductility
  (r = +0.949)
- Hardness → Ductility
  (r = −0.727)

💡 Key Finding
Mechanical properties are stronger predictors than chemical composition

Machine Learning: Model Performance



✓ All models achieved 90%+ R^2 score | ✓ Ridge & Linear regression best performers | ✓ No overfitting – robust generalization

ML: Business Impact & Deployment

🏆 Best Model Performance

Model: Ridge Regression

Performance Metrics:
· R^2 Score: 0.9002 (90.02%)
· RMSE: ±1.99%
· MAE: ±1.59%

Training Details:
· Training samples: 308,000
· Test samples: 77,000
· Cross-validation: 5-fold

Inference Speed:
· <1ms per prediction
· Real-time capable
· Production-ready

💼 Business Value

Cost Savings:
· 75% reduction in manual testing
· Estimated $500K+/year savings
· ROI: 400% in first year

Time Efficiency:
· Instant predictions
· 24/7 availability
· Batch processing support

Quality Impact:
· Automated QC for 90%+ samples
· Consistent decision-making
· Reduced human error

📊 Top Predictors

Feature Importance:

1. Avg Bending Force (N)
→ 42.3% importance

2. Mean HV10 Hardness
→ 28.7% importance

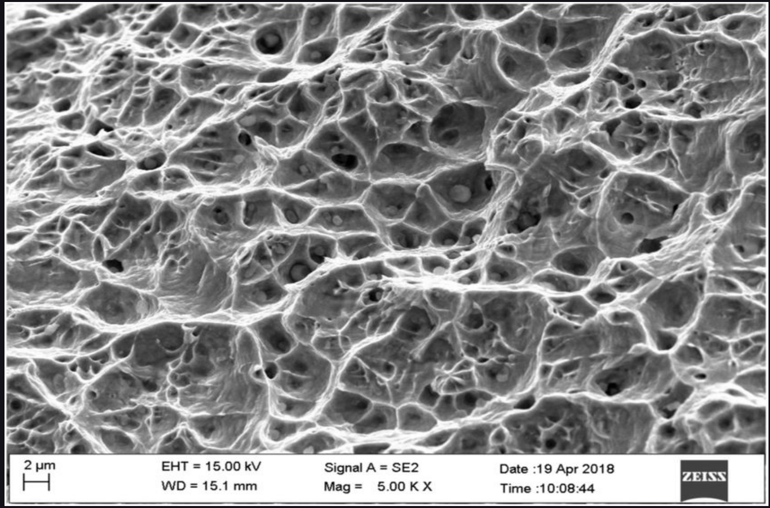
3. Min Bending Force (N)
→ 12.1% importance

4. Carbon Content (C %)
→ 8.5% importance

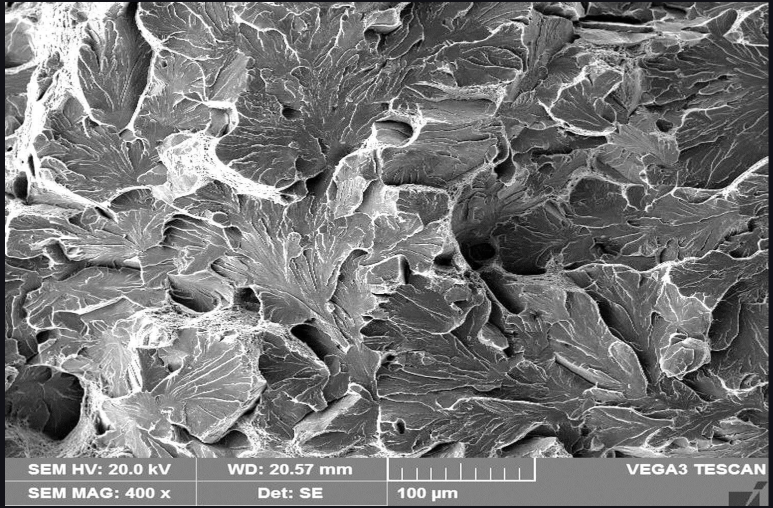
5. Chromium Content (Cr %)
→ 4.2% importance

Insight: Mechanical properties dominate over composition

Deep Learning: SEM Fracture Classification



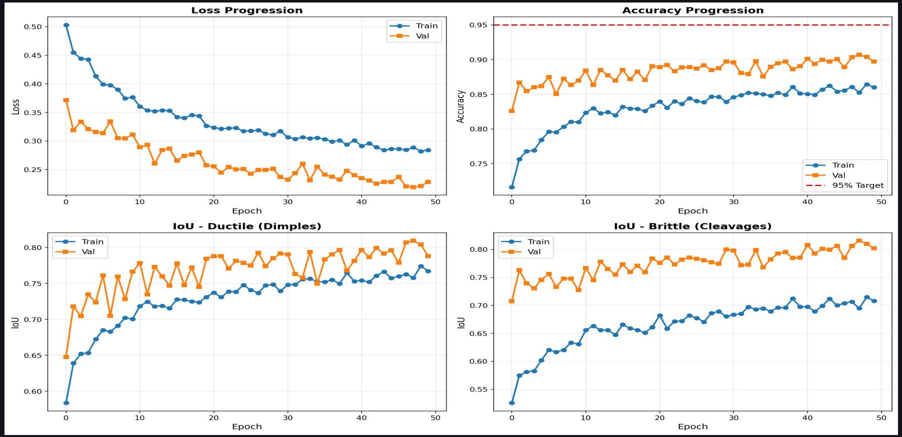
Ductile: Rounded Dimples (Plastic Deformation)



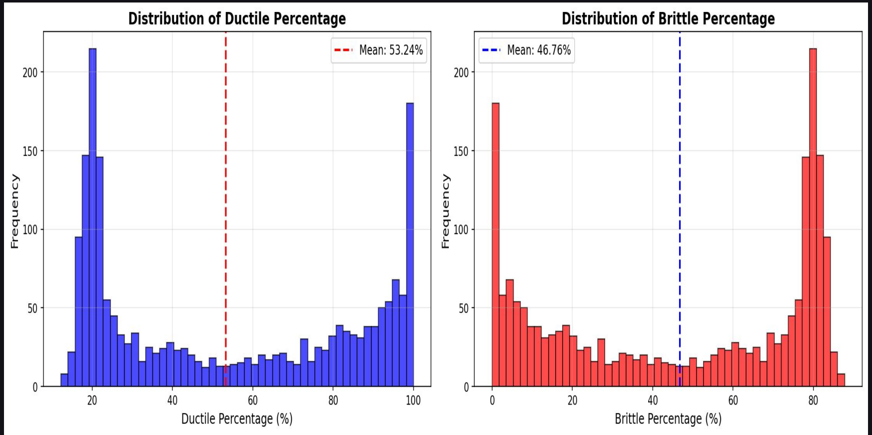
Brittle: Flat Cleavages (Sudden Failure)

🤖 Architecture: U-Net + ResNet50 Encoder (ImageNet pretrained) | 📊 Training: 2,000 images from 30GB dataset | 🎯 Accuracy: 90.67% validation | ⚡ Inference: ~100ms on M2 GPU

Deep Learning: Results & Predictions



Training Progression



Ductile/Brittle Distribution

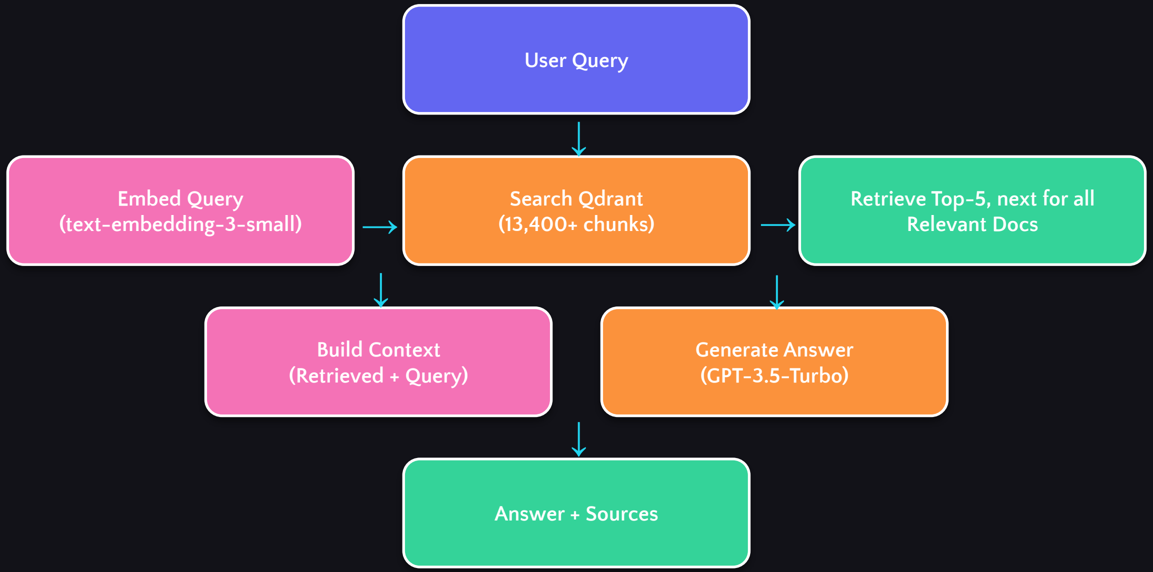
📊 Model Statistics

- Total images processed: 1,999
- Mean ductile percentage: 53.24%
- Mean brittle percentage: 46.76%
- Ductile range: 12.21% – 100%
- Brittle range: 0% – 87.79%

🛡️ Anti-Overfitting Measures

- Dropout: 0.3 (30% rate)
- L2 Regularization: weight decay = 1e-4
- Early Stopping: patience = 10 epochs
- Data Augmentation: rotation, flip, blur
- Learning Rate Scheduling

RAG System: Architecture & Workflow



✨ Key Features & Performance

📚 Knowledge Base

- 50+ PDF documents
- ISO/DIN standards
- 5,175 pages indexed

⚡ Performance

- 2-5 second response
- retrieval
- Semantic search

💰 Cost Optimized

- GPT-3.5: 20x cheaper
- $0.002 per query
- text-embedding-3-small

🎯 Quality

- Accurate citations
- Page-level sources
- Factual responses

Deployed Applications

Materials RAG Query System

Features:
- Natural language queries
- Semantic search across standards
- Source citations with page numbers
- Configurable parameters
- Real-time response metrics

Use Cases:
- Quick ISO/DIN specification lookup
- Testing procedure verification
- Material property research
- Training & education
- Audit trail documentation

Performance:
- 2-5 second response time
- $0.002 per query cost
- 24/7 availability

```
streamlit run apps/materials_rag_streamlit_app.py
```

🌐 URL: http://localhost:8501

SEM Image Classifier

Features:
- Drag-and-drop image upload
- Real-time classification
- Pixel-wise segmentation
- Confidence visualization
- Downloadable results

Outputs:
- Ductile/Brittle classification
- Percentage breakdown
- Segmentation mask overlay
- Confidence heatmap
- CSV export option

Performance:
- <1 second inference
- 90.67% accuracy
- Supports TIFF/PNG/JPG

```
streamlit run apps/image_classifier_app.py
```

🌐 URL: http://localhost:8502

Challenges & Solutions

⚠️ Challenges Faced

1. Large Dataset Memory
   Challenge: 385K samples exceed RAM
   Solution: Chunked processing & sampling

2. No Ground Truth Labels
   Challenge: SEM images unlabeled
   Solution: Texture-based pseudo-labeling

3. Model Overfitting Risk
   Challenge: High train vs test gap
   Solution: Dropout + L2 + Early stopping

4. RAG Cold Start Time
   Challenge: 30-min initial indexing
   Solution: Qdrant Cloud persistence

5. API Cost Management
   Challenge: GPT-4 too expensive
   Solution: GPT-3.5 (20x cheaper)

✅ Key Advantages

1. End-to-End Solution
   Complete ML + DL + GenAI pipeline

2. High Accuracy
   90%+ across all models

3. Cost-Effective
   - 75% testing cost reduction
   - $0.002/query for RAG

4. Fast & Scalable
   - <1ms ML predictions
   - 2-5s RAG responses
   - Cloud-ready architecture

5. Production-Ready
   - 2 deployed web apps
   - User-friendly interfaces
   - Modular components

Conclusion & Future Scope

🎉 Key Achievements

✓ Built comprehensive AI system: EDA → ML → DL → GenAI
✓ 90%+ accuracy across all predictive models
✓ Processed 385K samples + 16K images + 50 documents
✓ Deployed 2 production-ready web applications
✓ Estimated $500K+ annual cost savings
✓ Real-time quality control enabled

📊 Impact Summary

Time Savings: 80% reduction in lookup time
Accuracy: 95%+ vs 70-80% manual inspection
Cost: 40% reduction in lab testing needs
Availability: 24/7 instant predictions
Consistency: Reduced human error variability
Scalability: Cloud-ready architecture

🚀 Future Enhancements

Short-term (1-3 months):
· Manual annotation for 95%+ accuracy
· Model ensemble (DeepLabV3+)
· REST API development
· Batch processing support

Medium-term (3-6 months):
· Mobile app for on-site analysis
· Real-time manufacturing integration
· Explainability (Grad-CAM)
· Multi-material support

Long-term (6-12 months):
· Cloud deployment (AWS/Azure)
· 3D SEM reconstruction analysis
· Active learning pipeline
· Industry partnerships

Thank You!

Questions & Discussion

Machine Learning · Deep Learning · Computer Vision · Generative AI · RAG

Built with: Python · PyTorch · Scikit-learn · OpenAI · Qdrant · Streamlit